



Supplement of

Effects of dust particle internal structure on light scattering

O. Kemppinen et al.

Correspondence to: O. Kemppinen (osku.kemppinen@fmi.fi)

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This supplementary document provides more details on a few potential technical questions the reader might have: DDA accuracy with the chosen dipole resolution, the effect of particle variability within the three-particle ensemble used, and the choice of effective medium approximation.

1 DDA accuracy

We have employed the -jagged option of ADDA to study the inaccuracies related to shape determination. Unfortunately, even -jagged 2 consumes roughly 8 times as much CPU time, which would be almost one million CPU hours for the full runs, which would take several months with the computing resources available to us. Instead, we have decided to perform limited tests, and only for -jagged 2 (double dipole resolution along each axis, 8 times the total number of dipoles) instead of e.g. -jagged 4 (quadruple dipole resolution along each axis, 64 times the total number of dipoles).

To get as detailed results as possible while preserving computer resources, we chose two individual size parameters to study, x = 5 and x = 16. The results for these, comparing each inhomogeneous run to the corresponding EMA runs, are shown in Figures 1 and 2 below for all of the scattering matrix elements. We see that for x = 5, the difference in resolution produces negligible changes in scattering, whereas the effect of using EMA is very large. In the case of x = 16, for some scattering matrix elements the finer resolution makes a noticeable difference, comparable to that of using EMA. However, if the EMA particle is also simulated with the double resolution, the EMA error remains relatively constant to the original resolution cases. Therefore, while the absolute values become more accurate, EMA does not perform better.

We conclude that the dipole resolution used caused relative errors of 1-10% at large size parameters, depending on the scattering matrix element in question, and <1% at small size parameters, where most of the particle sizes are located at in our particle size distribution. In contrast, the large particles have relatively small weights: size parameters 16 and larger have only a combined weight of 2.4% in the ensemble. Regardless, based on this, extra care should be taken with wider particle size distributions, and while the main features of simulations are unlikely to change, double dipole resolution should be considered at x > 16 to reduce uncertainties.

As a final note, of the scalar scattering quantities considered, only the linear depolarization ratio is changed noticeably by double dipole resolution (which increases by 13% at x = 16 due to S_{22} sensitivity); all others are virtually unaffected.



Figure 1: Results of the double resolution experiment for size parameter 5, showing all of the scattering matrix elements and using one of three Case 2 particles. The difference in doubling the dipole resolution is insignificant in comparison to the EMA error.



Figure 2: Results of the double resolution experiment for size parameter 16, showing all of the scattering matrix elements and using one of three Case 2 particles. The errors by using the original resolution instead of the doubled one can be up to 5-10% for some scattering matrix elements, which is comparable to the EMA error. However, when EMA particle is also simulated with double resolution, EMA error stays relatively constant. For other elements, the dipole resolution error is very small, similarly to the smaller size parameters.

2 Shape ensembles

Here, we clarify the possible effect of using three-particle ensembles instead of studying single particles. In Figures 3 and 4 in this supplement we have shown Case 2 for two individual size parameters (6 and 18) where the standard deviation of the three particles is used as the error bar (one SD above the line, one SD below the line, i.e. the total bar covers 68% of the variability). Naturally, SD is not a very good measure when N=3, but it should give a scale of the variability nevertheless. Individual sizes are shown instead of size-integrated values to see the difference at different sizes. It is noteworthy that the strong oscillation seen at some of these values is due to using single sizes and goes away at size integration, and thus is unrelated to the particle-to-particle variability.



Figure 3: Scattering matrix elements for Case 2 ensemble at size parameter 5, with error bars added to denote ± 1 standard deviation variability of the individual particles in the ensemble. For most part, the variability is smaller than the differences between individual curves.

Additionally, we have added some variability quantification to the text. We decided not to include the error bars to the (grayscale) figures in the article to keep them clear, and because the ensemble variability is not the focus of the article. The ensemble mainly provides oscillation reduction in scattering matrix elements, but since the inhomogeneous ensemble is compared against the homogenized ensemble, the conclusions are unlikely to change even if we



Figure 4: Scattering matrix elements for Case 2 ensemble at size parameter 16, with error bars added to denote ± 1 standard deviation variability of the individual particles in the ensemble. For most part, the variability is smaller than the differences between individual curves.

were to compare individual inhomogeneous particles to corresponding individual homogenized particles.

3 Effective medium approximation selection

When testing the performance of EMA's, an especially when making a claim that EMA's (in general) can not replicate scattering, it is important to test different EMA methods and select the most appropriate one. Here, we test five different EMA's: normal and inverse Maxwell Garnett (MG), Bruggeman, volume average of refractive indices, and volume average of permittivities. Due to heavy computational costs we did not perform the full scattering calculations for all of these. Instead, we chose two cases, Case 2 and Case 5, to test, due to the fact that their hematite content likely has the greatest effect on EMA's. Additionally, instead of studying the size distribution integrated values, we study two individual sizes, x = 5 and x = 16, to see if and how the EMA validity changes as a function of the size parameter.

Case 2 is simplified by considering only 2 materials instead of the original 12, because the traditional MG is applicable to only 2 materials. We have thus chosen as the materials to study a bulk clay mineral with refractive index of 1.55 + i0 and volume fraction of 85%, and hematite with refractive index of 3.09 + i0.0925 and volume fraction of 15%. The EMA of this simplified system obtained by volume average of refractive indices is 1.78 + i0.0139, close to the original Case 2 EMA m of 1.78 + i0.0135. Because the clay minerals in the original inhomogeneous particles have very similar refractive indices (most of the minerals are within between refractive indices 1.52 and 1.57, with roughly 6% of the total volume having refractive indices of up to 1.60), and based on the close match in the homogenized refractive indices between the original and the simplified versions, we conclude that it is likely that this simplified case is representative of the original case.

We have chosen to replicate the results with five different EMA's using this simplified composition: the original way of averaging refractive indices (1.78 + i0.0139), averaging permittivities (1.86 + i0.0230), MG using larger volume fraction as the matrix (MG1, 1.73 + i0.0073), MG using larger volume fraction as the inclusion (MG2, 1.80 + i0.0172), and Bruggeman (1.74 + i0.0089). It is very important to note that the particles in this study are generally not within the validity criteria of the EMA's, which also may help to explain the results below. For example, the assumption that the inclusions are much smaller than the wavelength does not hold for the particles considered here. It could be argued that highly localized and spatially nonuniformly distributed inhomogeneity is very hard to represent by any simple parametrization, unless specifically tuned for each individual particle and even size parameter. These results are visualized in Figures 5 and 6 below for size parameters 5 and 16, respectively.

The results show that for x = 5, on average, all EMA's tested perform



Figure 5: Case 2 scattering matrix elements with different effective medium approximations for size parameter 5



Figure 6: Case 2 scattering matrix elements with different effective medium approximations for size parameter 16

extremely badly. It seems that inhomogeneity dampens the oscillations by reducing regularity.

For x = 16, the results are more varied, depending on the scattering matrix element in question. We do not go into detailed analysis here, but

the results can be summarized as follows. Overall, mean m and MG2 seem to be behaving the best, with MG1 and Bruggeman being the worst. Mean permittivity behaves optimally in some cases, such as small scattering angles of S_{44} , but badly in other cases. Furthermore, different EMA's give better matches at different scattering angles, which means that an EMA that works well at, say, backscattering direction, might not work well at all at other directions.



Figure 7: Case 5 scattering matrix elements with different effective medium approximations for size parameter 5

For comparison, we also tested another case, the one with thin hematiterich coating (Case 5), again simplifying the particle to only two components to allow MG to be used. The components were clay with m = 1.55 + i0.0 and volume fraction 82%, and hematite-rich clay mixture with m = 1.82 + i0.0139 and volume fraction 18%. The different effective refractive indices were as follows: mean refractive index: 1.60 + i0.0025, mean permittivity: 1.60+i0.0028, MG1: 1.60+i0.0023, MG2: 1.60+i0.0025, and finally Bruggeman: 1.60 + i0.0024.

The results are shown in Figures 7 and 8. Interestingly, the results differ from those of Case 2. First, all of the EMA's tested behave very similarly to each other for both of the sizes tested, as expected given the very closely matching refractive indices. This is likely due to smaller refractive index contrast in the two materials, compared to Case 2. Further, EMA's seem to work better at small size parameters than large size parameters; behavior at small size parameters is very decent, but at large ones the errors are tens



Figure 8: Case 5 scattering matrix elements with different effective medium approximations for size parameter 16

of percent. We speculate that this is likely due to thinness of the coating: at small size parameters the coating is too thin to interact strongly with radiation, which causes its effect to be modest and thus EMA's to work quite well. However, as the size increases and coating starts to have a larger effect, EMA's start producing wrong results.

Although only two cases and two individual sizes were tested, it seems safe to conclude that our findings related to the importance of explicit modeling of inhomogeneity does not depend on the choice of the EMA. Indeed, our choice was among the best for Case 2, i.e. the particle with hematite nodes, and likewise for Case 5 where all of the EMA's performed very similarly to each other. Since no EMA tested here seems to be behaving clearly better than the originally selected EMA, the conclusions of the article remain unaffected even if another EMA was selected.