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## ***Interactive comment on “Single scattering by realistic, inhomogeneous mineral dust particles with stereogrammetric shapes” by H. Lindqvist et al.***

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The manuscript provides an important step towards realistic simulations of light-scattering by atmospheric aerosols. It not only describes and successfully applies a new methodology, but also compares it with existing simpler approaches. The manuscript is well-written and is definitely worth publishing, but a few issues must be addressed before publication.

1) The authors state that their results can be used as a reference/benchmarks, and they deduct certain conclusions from comparison of their realistic simulations to sim-

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pler models. Thus, they should discuss the parameters and accuracy of the DDA simulations in much more details.

1a) The authors should describe the parameters of the DDA simulations in Section 4.2, at least the DDA formulation (is it LDR, the default in ADDA?), the  $dpl$  (number of dipoles per wavelength), and version of the ADDA code. Was the number of dipoles changing with size parameter? The authors should also specify the typical computational requirements (at least, for the largest particles). This can also explain/justify the upper limit of the size parameter, which was mentioned by another reviewer.

1b) It is important to control/quantify the simulation uncertainty. The author cite (Zubko et al., 2010) on p. 18463. However, it is unclear if it is a general reference, or if the authors adopt the convergence (accuracy) criterion from it. If the former is true, the authors should at least also refer to [Yurkin M.A. and Hoekstra A.G. The discrete dipole approximation: an overview and recent developments, J. Quant. Spectrosc. Radiat. Transfer 106, 558–589 (2007). <http://dx.doi.org/10.1016/j.jqsrt.2007.01.034> ], which contains a comprehensive overview of DDA accuracy in different cases. If the latter (adopting convergence criterion) is true, this is very arguable without additional justification, since results of Zubko et al. are rather specific.

Anyway the authors should explain why (based on what criterion) they used so many dipoles for the largest size and quantify (at least roughly) the accuracy of their simulations. The methods to do it are described, e.g., in Section 2.1 of (Yurkin and Hoekstra, 2011), based on simulation of the same particle with different dipole sizes. The largest number of dipoles ( $10^5$ ) is not that large (even considering orientation averaging), so substantially refining the discretization (decreasing dipole size at least 2 times) should be computationally feasible for several representative examples. Especial care is required for backscattering quantities, since DDA with default parameters may calculate them with large errors in certain cases.

1c) The authors should specify the orientation-averaging scheme in Section 5.2 addi-

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tionally to the plain number of orientations. Is it the built-in scheme of ADDA? If yes – what is the number of alpha, beta, and gamma angles? Why those numbers were selected, what is the estimated uncertainty (of different computed quantities) due to orientation averaging? If ADDA's scheme is used, the raw output does contain estimates of this uncertainty.

2) The missing element in the whole approach (important for validation) is measurements of the scattering from single particles. The authors correctly mention that no such measurements has been made for these specific particles. However, there exist techniques potentially capable of performing such task, although coupling these systems with the shape reconstruction of the same particle is not easy: Air flow systems measuring 2D scattering patterns – developed by Kaye et al. See the review in [Kaye P.H., Aptowicz K., Chang R.K., Foot V., and Videen G. Angularly resolved elastic scattering from airborne particles, in *Optics of Biological Particles*, eds. A.G. Hoekstra, V.P. Maltsev, and G. Videen, Springer, Dordrecht, pp. 31–61 (2007). [http://dx.doi.org/10.1007/978-1-4020-5502-7\\_3](http://dx.doi.org/10.1007/978-1-4020-5502-7_3) ] Air flow systems measuring holographic patterns – see e.g. [M. J. Berg and G. Videen, Digital holographic imaging of aerosol particles in flight, *J. Quant. Spectrosc. Radiat. Transfer* 112 p. 1776-83 (2011). <http://dx.doi.org/10.1016/j.jqsrt.2011.01.013> ] (Liquid) flow cytometers, measuring 1D and 2D scattering patterns: [Strokotov D.I., Moskalensky A.E., Nekrasov V.M., and Maltsev V.P. Polarized light-scattering profile - advanced characterization of nonspherical particles with scanning flow cytometry, *Cytometry A* 79A, 570–579 (2011). <http://dx.doi.org/10.1002/cyto.a.21074> ] [Jacobs K.M., Lu J.Q., and Hu X.-H. Development of a diffraction imaging flow cytometer, *Opt. Lett.* 34, 2985–2987 (2009). <http://dx.doi.org/10.1364/OL.34.002985> ]. So the authors should discuss (some of) these techniques in the introduction and, probably, in the discussion or conclusion with respect to possible future work.

Finally, a minor comment – the authors may consider pointing out in the Introduction an analogy between their approach to mineral aerosols and the realistic modeling of

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light-scattering from biological particles, based on confocal images. See e.g. [Brock R.S., Hu X., Weidner D.A., Mourant J.R., and Lu J.Q. Effect of detailed cell structure on light scattering distribution: FDTD study of a B-cell with 3D structure constructed from confocal images, J. Quant. Spectrosc. Radiat. Transfer 102, 25–36 (2006). <http://dx.doi.org/10.1016/j.jqsrt.2006.02.075> ] and [Orlova D.Y., Yurkin M.A., Hoekstra A.G., and Maltsev V.P. Light scattering by neutrophils: model, simulation, and experiment, J. Biomed. Opt. 13, 054057 (2008). <http://dx.doi.org/10.1117/1.2992140> ]

Interactive comment on Atmos. Chem. Phys. Discuss., 13, 18451, 2013.

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