Second review of « A generalized photon-tracking approach to simulate spectral snow albedo and transmissivity using X-ray microtomography and geometric optics », by Theodore Lechter et al.

General comments

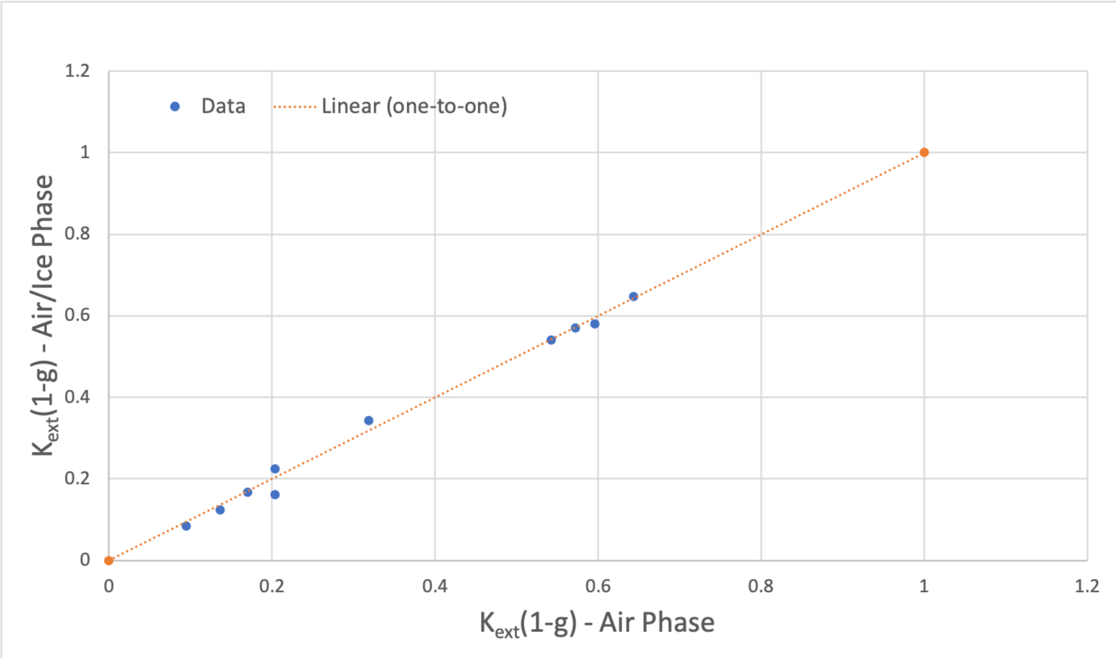
Much effort have been made to improve the scientific quality and the clarity of the manuscript, which has been significantly revised compared to the initial version. New figures have been appended, and many others were updated. This is appreciated and certainly makes this study more convincing. However I believe an additional effort is still required to make it an even more significant and scientifically robust contribution. In particular, issues that have been partly tackled in the response to reviewers should be further tackled and included in the paper. These issues are detailed below.

Specific comments

1) The most questioning remaining issue concerns the definition of extinction coefficient for a porous medium. It is explained in the text (and in more details in the response to reviewers) that the computed extinction coefficient does not perfectly match the expected dependence (from theory on particulate media) on SSA and density. This is attributed to the way extinction coefficient is computed, with photons launched from anywhere in the medium, and not only in the air (which is what is implicitly done when launching photons on an isolated ice particle in air). I believe this raises a very important question about the definition (if only it means anything) of the extinction coefficient for a porous medium. In particular with this method the authors find for a collection of spheres a value of the extinction coefficient different than the commonly accepted value. What is the meaning of having different extinction coefficients, when such a quantity should be intrinsic to the medium? This critical question cannot be overlooked, otherwise your method could be erroneously replicated by others. My guess is that defining extinction coefficient and phase function (and probably absorption along extinction paths along with those two quantities) for a porous medium is not univocal, and definitely not trivial. Clearly there exist alternative strategies that result in different values. However I think that for radiative transfer what matters is the product $\gamma_{ext}\cdot(1\text{-}g)$, which is probably the same for any strategy (also explaining why the computed albedos satisfactorily match). Hence I would recommend to estimate γ_{ext} in the common way (launching photons from the air phase only) and to compute the phase function using the deviation between entrance angle (into the ice phase) and final escape angle (after some internal reflections). Applying this to a collection of spheres would help check whether accepted values are retrieved for the phase function (or g) and extinction coefficient, and whether both strategies are indeed equivalent for radiative transfer. Actually you can already check whether $\gamma_{ext}\cdot(1\text{-}g)$ obtained with your method for the collection of spheres matches the "particle approach" value. This is certainly beyond the initial scope of this paper, but the strategy proposed cannot really be accepted before it is proved that it replicates exactly (regarding this, care should be taken to ensure that the obtained match is convincing, which was not the case in the new figure of spectral albedos provided in the response to reviewers) what is expected for a collection of spheres. Tackling this issue would strongly support the presented strategy, and would be a major contribution to radiative transfer in snow (actually in any weakly absorbing porous medium).

We thank the reviewer for this thoughtful and engaging question. In response to this question, we undertook a major effort to track down the discrepancies between various approaches and ultimately reassessed how to get the extinction coefficient for our model. The outcome of this is summarized here.

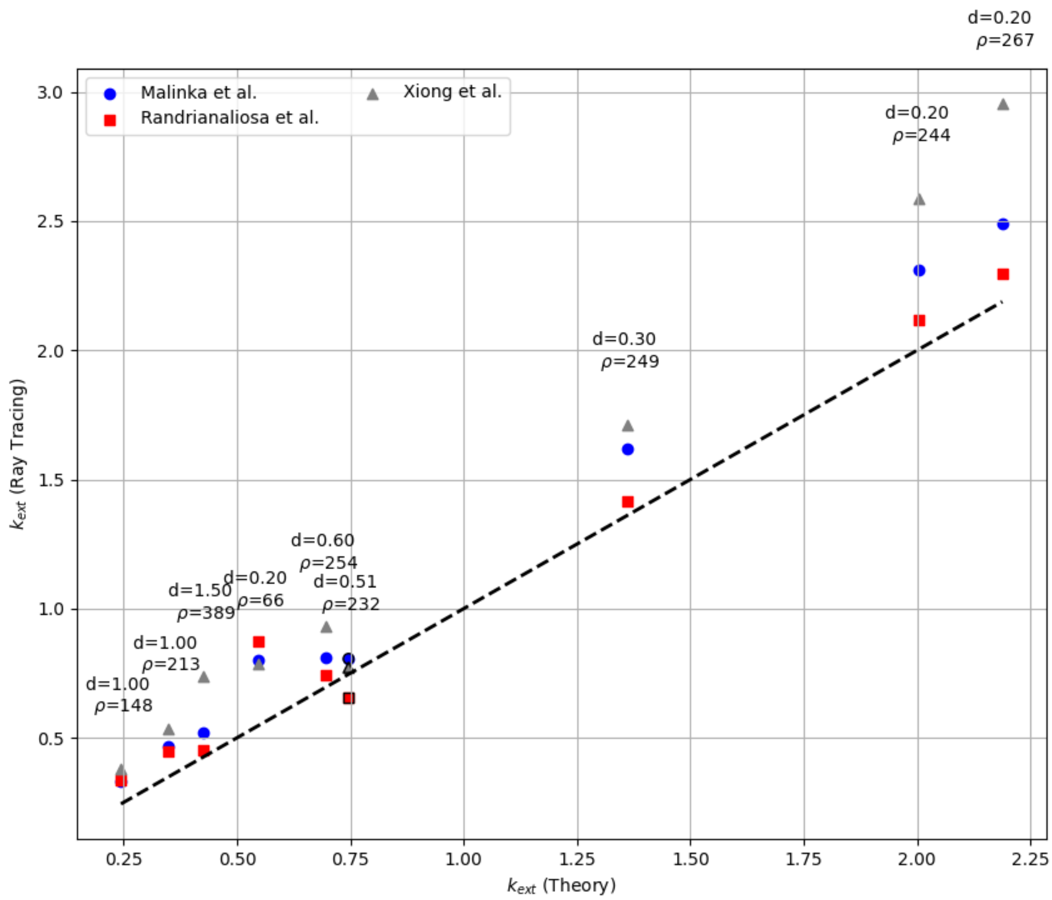
1. First, a limited assessment comparing the inverse-transport length [γ_{ext}*(1-g)] computed for a selection of spheres with photons initialized in the air phase only and the asymmetry parameter from the "whole particle" scattering does indeed match with γ_{ext} computed with photons initialized in both phases and the "localized" scattering. This result would support the hypothesis posed in the discussion part of the previous draft (see figure below).



2. A more robust comparison of a variety of different methods for computing γ_{ext} through ray-tracing methods and an additional literature review suggest that:

   a. The Xiong et al. (2015) method of initializing particles at random positions throughout the medium is not entirely consistent with the definition of the extinction (scattering) coefficient as the inverse of the mean distance traveled between scattering events. In essence, because the particles are not by necessity initialized at a scattering event (particle boundary), the extinction coefficient is artificially high following this method. This is explicitly stated in Randrianaliosa and Ballis (2010). Further, through additional work, we were able to determine that the curve fitting used by Xiong et al. (2015) is largely unnecessary, as it will converge to generate a γ_{ext} that is equal to simply 1/mean free path.

   b. In following the points illustrated in (a), we have decided that the Xiong et al. (2015) method for determining the extinction coefficient has some potential issues with it that we hadn't fully grasped until diving deeply into it, and while it may work in some instances, we think it would be better to choose a more reliable method. Accordingly, we have decided to compute the extinction coefficient following the method in Randrianaliosa and Ballis (2010), which simply computes the extinction (scattering) coefficient from the mean path length between scattering events during the ray-tracing step. In this method, scattering events are defined with respect to the whole particle, such that internal reflections are not counted as discrete events. Scattering events only occur when the ray enters or exits the particle via either reflection or transmission. We feel that this method is more robust and more consistent with the medium based model. Further, in a comparison of different methods for computing γ_{ext}, we find that the Randrianaliosa and Ballis approach reproduces the SSA*rho/4 better than other methods. (see below scatter plot)



Scatter plot of γ_{ext} for various ray-tracing techniques plotted against theory.
Note that the Xiong et al. technique here is for particles initialized in the air-phase.

c. Because this framework defines scattering events with respect to the whole particle, we have accordingly opted to use to the "whole particle" phase function as well. This is computed using the entire sample, such that segmenting grains is not required.

d. All of the methods compared in this latest round of reviews (Xiong et al. 2015; Malinka et al., 2014; Randrianaliosa and Ballis, 2010) produce a large spread in results (see above), showcasing the difficulty in estimating optical properties through ray-tracing techniques. While tracking down the reasons for this would be a worthwhile endeavor, we feel that doing so is beyond the scope of this work. We speculate that there are several nuanced differences between the methods that are responsible for the differences, e.g.: random vs. controlled transport paths, the role of total-internal-reflection traps. However, we haven't performed a more in-depth investigation into this as of yet. We do, however, note that others have remarked on some of the uncertainty in understanding and estimating the extinction coefficient for snow (e.g., Malinka et al. 2014).

e. All in all, we think that a large source of this uncertainty that we have struggled with is because the Xiong et al. (2015) method treats scattering events differently than other approaches, with respect to how both the mean free path and extinction coefficient and phase function are treated. We would like to note that when updating our model such that scattering events are more similar to the most common understanding, the changes to our results in the plane-parallel were almost negligible. So we speculate that the Xiong et al. 2015 method may be fundamentally consistent with other approaches. However, we are unable make this claim definitively, and have chosen not to as part of this work due to significant and non-intuitive/unexpected nuances involved on the computer-science side. Accordingly, we have opted to stick with more accepted definitions. We have added a paragraph to the discussion on this point and indicated that this model can be used to further investigate.

2) Some figures (e.g. spectral albedo in Fig. 13 (now Fig. 10)) and values (e.g. Table 1) have changed between both versions, while they apparently correspond to the same measurements, which is puzzling. It would be helpful to explain these differences (at least for the reviewers).

Response: Not providing an explanation for this change in the first round of revisions was an oversight on my part during the first round of reviews. In short, we had identified a minor coding error in our script used to plot the spectral albedo that pointed to incorrect reference scans for the 4.5 and 2.5 cm albedos. We also made a minor downward adjustment to the reflectance value of the reference panel as a majority of clean-snow reflectance's exceeded 1 in the blue-visible spectrum. To this point, all code and observational measurement and metadata used to make these figures will be included with the code repository on GitHub.

<u>Technical comments</u> (lines correspond to the track changes version)

l.16: the RMSE value might not be meaningful here, because it depends on the number of samples considered, on the characteristics of snow, on, the spectral range of the measurements… which are not detailed. Also, reflectance is rather "measured with a spectroradiometer" than "estimated".

Response: Thank you, we have revised the text to include the spectral range of the measurements for greater context. The remaining information is detailed in the body of the article. The recommended change in wording from "estimated" to "measured" was also made.

l.92: this long paragraph is surprising because it already contains much information, especially about the second component of the model. Shouldn't a large part of it (after l.98) be moved to the subsections?

Response: Thank you for this suggestion. We have shortened this paragraph and merged most of the information contained within it into the sub-section describing, in detail, the plane parallel model.

l.95: should the term "ray-tracing" or something equivalent appear here? Actually both models are somehow based on ray-tracing

Response: Thank you for the suggestion, this has been reworded as part of the l.92 response.

l.113: could you expand on why "the semi-quantized approach described here reduces the number of photons required to achieve a statistically robust result"

Response: We had used the phrase "semi-quantized" to help specify that photon-tracks were considered discrete (i.e., quantized) while the absorption was treated continuously. However, in some of the rewording/reorganizing of the paper, we have removed this phrasing, so it is no longer an issue.

l.116: "in this model": is it in the first or second component that phase and diffraction are ignored? I'd rather say in the first component, since the second component just takes as inputs statistically representative single scattering properties, no matter where they come from

Response: Thank you for this clarification. To be more specific, we have rephrased this sentence as: "*One critical simplification we make in determining the optical properties of a given snow sample is that we ignore the wave properties of light …"*

l.136: isn't "a photon of light" redundant?

Response: Yes, good catch. We have revised.

l.140: ice-path fraction or mean path fraction traveled within ice? Maybe chose a single consistent term.

Response: Thank you for the suggestion, we have replaced "mean path fraction within ice" with ice-path fraction.

l.143: the choice of starting anywhere in the medium (ice or air) seems (according to the author comments) to be the reason for not matching the expected relationship between extinction coefficient, SSA and density. Starting the paths only in the air would definitely change the obtained extinction coefficient (and the phase function accordingly). So it raises a fundamental question about how to define the extinction coefficient of a porous medium, which may be an ill-posed question. See specific comment 1).

Response: This is a question that we have been grappling with since going over the initial reviews.

We refer you to our more in-depth response to comment 1. However, we do reiterate here that there is significant ambiguity regarding the definition of the scattering/extinction coefficient in porous media. In particular, scattering events can be defined either as occurring over a whole particle, or at the dielectric boundary comprising the particle surface. While traditional RT methods and theory accept the former, ray-tracing is well suited to the latter, and we were not able to find any published research that truly attempted to reconcile these approaches. The method from Xiong et al. 2015, follows the latter method, which is one reason we speculate that it does not reproduce theory under idealized conditions. Furthermore, this method, whereby particles are initialized *at random* throughout the medium as opposed to on air/ice boundaries is explicitly discounted as wrong by Randrianalisoa and Baillis (2010). Further, Malinka et al. (2014) suggests that the definition of the extinction coefficient is not entirely settled and that there is no rigorous proof that the forms in Van De Hulst (1957) and Kokhanovsky and Zege (2004) hold true for random mixtures and dense-packed media. So, while there definitively seem to be fundamental unanswered questions regarding scattering in the extinction coefficient in porous media, we feel that trying to answer them here is beyond the scope of this work. Accordingly, have reverted to a method that is most consistent with accepted theory due to outstanding issues and growing skepticism towards the Xiong et al. (2015) method that we had used initially. We do want to note that while the optical properties generated from the Xiong et al. (2015) method are quite different from the optical properties generated from other methods, the actual simulated spectral albedos computed from each set are almost indistinguishable, at least for the simulations discussed in this study.

l.215: consider providing here (or in the caption of Figure 2) the number of photons used to compute these statistics. Also the exponential fit does not seem very convincing. Discussing errors in this fitting procedure (fitting for instance the log of the POE) would be useful. To which extend could this uncertainty of the fit explain discrepancies with the usual dependency on density and SSA?

Response: We have included the number of photons in the caption for figure 2. We have included a response made to a similar comment from another reviewer on the first round of revisions that discusses some of the uncertainty in the curve fitting procedure below. While the actual uncertainty in the curve fitting procedure is generally small, it doesn't always match the POE. However, in light of the response to the first major comment, the curve fitting procedure is moot, since it is no longer used.

Previous Reviewer Response: The uncertainty for a given value of the extinction coefficient is very low for set parameters. For example, repeating the calculation of it for the same sample, same wavelength, and same curve fitting technique yields a standard deviation of <0.05 if enough photons are used (>2000 seems to be sufficient for convergence). However, there is more substantive uncertainty if the parameters that influence the curve fitting are modified. For example, if the distance sampling is different, or if the initial guess that feeds into the curve fit is modified can yield differences as high as 0.3.

Figure 1: a) ke in the legend should have a unit. By the way what is ke? In the Figure caption refer to a, b, c, d. c) what is the dashed red line? d) 1000 nm should be in the suptitle rather than in the legend

Response: Thank you for catching some of these inconsistencies from previous revisions. We have made all of the suggested updates to the figure and the figure caption. We removed the 1000nm remark entirely, and instead note in the methods section that we assume an index of refraction of 1.30.

l.260: still, I think this Eq. (17) implies that the total physical length traveled by the photons is the sum of the s segments, while due to the internal reflections quantified by the B parameter a longer total distance is traveled, so that s should be scaled accordingly

Response: We think that this question is part of the same ambiguity surrounding how scattering events are defined and quantified with the extinction coefficient and scattering phase function highlighted in previous comments. For instance, if internal scattering events are considered distinct when computing the extinction coefficient, an internal path extension would not be required. However, now that our methods are more closely aligned with currently accepted definitions, it is clearer that an adjustment to Fice is needed to account for this. In revisiting this from an analytical standpoint, we can show by combining equations from Libois et al. 2014 and Libois et al. 2019 that the absorption coefficient can be expressed in terms of Fice as -> $\sigma = F_{ice}\left(1 + \frac{\rho_s}{\rho_{ice}}[B-1]\right)\gamma$. Accordingly, the scaling of the "s" length for equation 17 for absorption when computing it through F_{ice} is close to 1 (1.02 - 1.15) for most samples. We have added this scaling to the absorption function used in the plane parallel model, and more explicitly described how the "B" parameter is computed, since it is now a critical optical property used in the plane-parallel model. However, we do note that there are some outstanding uncertainties surrounding this parameter that seem to be related to the fact that it's being calculated within a sample comprised of a collection of snow grains, rather than a single particle. We have included some text on this in the discussion.

l.280: Figure 2

Response: Fixed, thank you.

l.339: one tenth rather than 10 times?

Response: Thank you for catching this typo, we have revised the text to one tenth.

Figure 5 caption: different types of what?

Response: Thank you for catching this typo, we have completed the sentence with "...types of snow grains."

Tables 1 and 2: could the g values (of the computed phase function) be indicated as well?

Response: Yes, see updated tables.

l.40: is it obvious what an exponential increase means? Maybe provide the functional form of the dependence

Response: We have replaced this sentence with: ***"This analysis shows an increase in albedo at high zenith angles that is most pronounced in the NIR that represents the functional dependence between albedo and cos(θ). This result is broadly consistent with results from previous studies that compare snow albedo and zenith angle."***

l.412: the definition of transmittance is ambiguous here. "Within a snowpack" suggests that the snowpack is thick and that the downward flux is estimated at an intermediate depth, rather than at the bottom of the snowpack. Please clarify this, because both quantities (e.g. flux below a 5 cm layer and flux at 5 cm depth in a thick layer) are very different.

Response: We have clarified this by rephrasing the sentence on Line 323 to say: ***"To accomplish this, the optical properties of the μCT samples in Fig. 7 are used to simulate and compare the downward flux at varying depths (Fig. 11)"***

Table 2: depth should start at 0 at the surface no?

Response: This is a bit tricky, in that while we agree that "depth" with the snow surface set as 0 is technically correct, we often think of it as increasing from the ground as zero when we refer to snow depth. Accordingly, we would like to leave this as is.

l.474: it would be worth commenting the fact that the scaling of Eq. (21) is not 0.5 as would be expected from the studies cited above

Response: There is a detailed discussion of this in the Discussion section of the manuscript. See previous comments regarding the extinction coefficient and updated results. While we are not getting exactly ¼*SSA*rho, the new mean-free-path method is much closer.

l.477 : not clear why rounded grains are supposed to have highest B values. Spherical particles have a low B compared to fresh, supposedly fractal snow.

Response: Thank you for this comment. In this instance, while we were able to sample fresh snow, we did not measure a good sampling of dendritic or fractal grains with the microCT. However, we note that the relationship between grain form and B was not clear, and that the clearest relationship was to see higher B values for smaller grains, which happened to be round (or at least roundish) as a majority of the larger grains were faceted or broken. In the ray tracing framework employed here, we find that photons are consistently more likely to get "trapped" in total internal reflection with smaller rounded particles, than they are for larger, more irregularly shaped particles, which we suspect increases the internal path length. We have rephrased this sentence to be clearer with respect to what our results show within the context of previous work:

"We note that there is no significant relationship between B and snow grain form or size, however there is a general tendency for B to be highest for samples with higher SSA and smaller grains which is qualitatively consistent with Kokhanovsky and Zege (2004) and Libois et al. (2014). However, due to limitations in the variety of snow samples and MicroCT resolution we are unable to make any concrete conclusions regarding relationships between B and grain form."

l.481 (367): as both γ_{ext} and F_{ice} depend on density, what is the meaning of varying them independently?

Response: The purpose of this was to assess the relative sensitivity of transmittance to each property independently. While certainly they are somewhat linked through snow density, we think it is important to include this sensitivity to illustrate that a) the transmittance depth is more sensitive to the extinction/scattering coefficient, and b) that the sensitivity to Fice is also dependent on the scattering coefficient (e.g., it is more sensitive to Fice for a low extinction coefficient). Also, because the extinction coefficient is also a function of SSA, it seems plausible that these combinations of γ_{ext} and F_{ice} could exist.

Figure 13: extinction coefficient should have units mm^{-1}. What do the points correspond to?

Response: Thank you for this catch, we have corrected the figure caption. Each point corresponds to a sample within that snow layer. We have added additional text in the figure caption to clarify this.

l.496: was it clearly stated how F_{ice} depends on B (when density is fixed)?

Response: We are not sure what statement this refers to since the line numbers provided do not align with those in the submitted manuscript. Without additional context, it is difficult to discern what the reviewer is referring to. However, we have included some additional discussion regarding the relationship between B and Fice that shows this dependence.

l.531: it should be made clear that the refractive index is taken constant only for the optical properties computations, not for the absorption modeling

Response: Done, thank you.

l.532: another point regarding the MIR is that radiative transfer should not be applied this way to dense media (shadowing effects are ignored while they are obvious when snow grains touch each other). It's actually a chance that the dilute media theory applies that well to snow (see Kokhanovsky (2004) for more details) but this holds only as long as snow is weakly absorbing, which is not the case anymore beyond 1400 nm. Likewise, surface features (the topmost few mm) matter in this spectral range, while they are probably not captured by manual measurements of snow.

Response: Thank you for bringing up these additional points. We have added text to the discussion covering these additional sources of uncertainty.

l.546: the term Monte Carlo is ambiguous because to me the estimation of the optical properties is also based on a Monte Carlo method (ray-tracing with various possible paths)

Response: We have revised the text to the following for clarification: ***"A primary goal of this modeling approach is to expand upon previous approaches aimed at incorporating 3D renderings of real snow microstructure into radiative transfer models for snowpacks of arbitrary depth, while maintaining the ray tracing methods utilized in the original Kaempfer et al. (2007) model."***

l.556: it's not clear why this work would help with subnivean hazards. In the introduction or here it would be nice to clarify what kind of features could be seen (or not) through the snow, and why knowing the snow transmittance can help

Response: We have modified this phrasing to remove subniviean hazards in replace it with: "***improved capabilities for determining the optical properties of shallow snowpack".***

Reference:

Kokhanovsky, A. A. (2004). *Light scattering media optics*. Springer Science & Business Media.

Randrianalisoa, J. and Baillis, D.: Radiative properties of densely packed spheres in semitransparent media: A new geometric optics approach, Journal of Quantitative Spectroscopy and Radiative Transfer, 111, 1372–1388, 2010.

Malinka, A. V.: Light scattering in porous materials: Geometrical optics and stereological approach, Journal of Quantitative Spectroscopy and Radiative Transfer, 141, 14–23, 2014.