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

This paper describes a novel approach to extract relevant snow optical properties, namely the mean fractional ice path, extinction coefficient and phase function, from X-ray microtomography samples. Using these optical properties, a plane-parallel Monte-Carlo radiative transfer model is run to simulate the reflectance and transmittance of a multi-layer snowpack. This blended model is first applied to a single layer ideal snowpack, and then to a real, layered snowpack that was probed on 12 February 2021 at Union Village Dam in Thetford, Vermont. For this snowpack, along with the snow samples, spectral reflectance measurements were performed above the snowpack, including mesurements with a black panel inserted at 2.5 and 4.75 cm below the surface. This model reproduces the expected sensitivity of transmittance and reflectance to snow SSA, as well as the strong anisotropy of snow reflectance. The comparison between simulated and observed reflectance is satisfactory, although large discrepancies remain in the near-infrared, which are attributed to deficiencies in the estimation of the phase function.

The paper is well written and the figures are clear. The topic perfectly fits in the scope of The Cryosphere, and estimating local optical properties from X-ray microtomography snow samples is certainly a question that deserves more research. The development of a new approach and its tentative validation with in situ measurements is a great contribution to tackling this question. In that sense this paper contains sufficient original material to be considered for publication. However, several critical issues remain, mostly regarding the estimation of snow optical properties, that preclude accepting the paper before major revisions are performed. The experimental validation step is not very convincing yet, and the discussion does not sufficiently dwell on the obvious limitations of the present study. As a result, the reader is let with poor confidence that the proposed model can reliably simulate snow optical properties, including transmittance which is the focus of the paper but is not supported by any experimental validation.

Specific comments

1) The phase function of the snow is estimated by first isolating individual snow grains, and using a ray-tracing code to estimate their single-scattering properties. Although there is probably no easy way to estimate the local phase function of a bicontinuous medium, this approach is very questionable. First there is no evidence that a snow sample can be separated into individual grains without making very arbitrary choices. Think for instance of old snow that resembles more a porous medium than an ancient collection of individual snow particles. Second, the number of such grains to be selected is not discussed while it is clearly a limitation of the approach. The approach proposed by Xiong et al. (2015) to estimate the phase function of a bicontinuous medium is more aligned with the strategy used to estimate the extinction coefficient, and could probably at least be compared to the current approach. Approaches used in other disciplines (scattering in any porous medium) may also provide interesting alternatives (see for instance Haussener et al., 2012). In addition, it would be great to provide the values of the asymmetry parameter computed for the estimated phase functions, which would allow comparison with usual assumptions made on this hardly measurable quantity.

2) A method is proposed to estimate the extinction coefficient of snow from the 3D images, which is based on sampling the probability to be scattered or absorbed when traveling a certain distance from a variety of locations chosen randomly. This strategy seems acceptable, but does not reproduce the dependence of γ_{ext} on SSA and density ρ expected for a collection of individual convex particles, that is $\gamma_{ext} = \rho \cdot SSA / 2$. This simple relation has been used in recent, similar, studies, though

(Malinka, 2014, Picard et al., 2016). Although this deviation from the expected behavior is already seen in the original paper by Xiong et al. (2015) (their figure 4c), it should be further investigated. For instance it would be worth checking that the present strategy reproduces the expected dependence in the case of a collection of spheres. If it were carefully confirmed that in real snow the relation $\gamma_{ext} = \rho \cdot SSA / 2$ does not hold, this would be an important result. Not also that Figure 14 should be recomputed, looking for a correlation between γ_{ext} and the product $\rho \cdot$ SSA.

3) To my knowledge, the use of the mean fractional ice path F_{ice} is quite unique to this study. Generally, the medium is instead represented by its absorption efficiency, or equivalently by its single-scattering albedo. In Eq.18, the energy of the photon packet is decreased along the path *s* due to absorption within the ice. However the distance traveled in the snow is underestimated when using a continuous representation, because the distance l_{ext} between scattering (or absorption) events is less than the actual distance traveled, which should include internal reflections not accounted for in l_{ext} (see Malinka 2014). As a consequence I believe (this has to be verified) absorption is overall underestimated with the present method. This can be easily corrected by carefully taking into account internal reflections (as is made for the estimation of F_{ice}). Hence I'd encourage the authors to compare their approach to a more standard one based on single-scattering albedo (in which case absorption is seen as a probabilistic localized event rather than a continuous process). This would help validate the F_{ice} approach or point to fundamental and critical differences between both approaches. Also, it should be physically explained why a linear relation is expected between ρ and F_{ice}.

4) Related to the previous point, I stress that some work has been focused in the past decade on the estimation of the absorption enhancement parameter B of snow (Libois et al., 2013, 2014, 2019), which is actually directly related to the proposed definition of F_{ice}. Estimations of B from the joint values of F_{ice} and ρ provide results quite different from those obtained elsewhere, which at least deserves comments, if it does not help pointing to deficiencies of the present study. Although this could in itself form relevant material for an independent, complementary study, it appears necessary to at least clarify this point.

5) The paper tries to differentiate from previous similar studies by focusing on transmissivity, in complement to more widely explored reflectance properties. However, only a few observations (practically, 3 reflectance spectra) are used to validate the model, which do not correspond to the primary focus of the work. Since these measurements are not very well simulated (compared for instance to those reported by Carmagnola et al., 2013), it does not give confidence in the transmissivity simulations, in particular in the near-infrared. We also note than in the visible some differences remain that could be partly explained by the presence of light-absorbing impurities, which is not really discussed.

6) One of the main problems of this paper is that it lacks a proper, critical discussion. In the current version the discussion is 15 lines long and does not really question the whole results of the paper. I'm convinced that given the uncertainties arising from the chosen method to estimate local optical properties, the issues related to the spatial representativity of the very small samples, and the very limited number of observations that unsuccessfully try to support the model, a much longer discussion would be very useful.

Technical corrections

l.3 : "based on X-ray microtomography" is unclear → "reflectivity of snow samples based on X-ray microtomography images ?

l.6 : is really the focus more on transmissivity than albedo?

l.7 : sub-nivean hazard detection is mentioned in the abstract but not later on

l.8 : should snow grain size be replaced by SSA? Because the advantage of having 3D images of snow samples is to get rid of the simple, unrealistic, granular approach

l.10 : not clear whether in the field transmissivity and/or reflectivity measurements were performed

l.13 : “is limited to the top 5 cm” and “can penetrate” is awkward. Transmissivity is a property. Should be rephrased.

l.14 – 15 : I think this result is quite obvious. Maybe consider providing another more specific result.

l.28 : “aggregate” is unclear

l.42 : to state that geometric optics works well some hint should be given about the typical size of scatterers in snow (or referring to a paper stating why it works well)

l.43 : I think the interaction between a “snow particle” and light is far from being well understood. Because we essentially don’t know what a snow particle is. Consider rephrasing the sentence.

l.47 : Here Mie theory is mentioned which seems to contradict the fact that geometric optics is used. Outside of the Mie regime, using a Mie code is probably useless.

l.49 : I’d say that Mie theory CAN ONLY BE (by definition) applied to spherical particles

l.53 : please double-check that the errors highlighted by Dang et al. (2019) indeed result from the spherical hypothesis, and not from the two-stream approximation

l.59 : Is it similar to the approach of Malinka (2014), which could then be cited as well?

l.62 : I’m not sure in Dumont et al. (2021) they used ray-tracing on numerical samples to simulate optical properties.

l.65 : I’d encourage the authors to use reflectance/transmittance (the measured quantity) or transmissivity/reflectivity (the material property), but not a mixture of both.

l.72 : I understand that the main difference of this study with the previous ones upon which it builds is the special focus on transmissivity. If it’s the case, consider being even more specific on this point.

l.75 : what does “semi-quantized” mean?

l.89 : “RT through non-spherical properties” is unclear. Do you mean to simulate single scattering properties of such particles?

l.83 : again, is the reference to Dumont et al. (2021) appropriate?

l.90 : remove “medium”

l.92 : how does this resolution compare with previous studies? Is it estimated to be sufficient to represent small-scale snow features that can have an impact on snow optical properties?

l.92 : does “1D” mean plane-parallel, that is horizontally homogeneous layers? Maybe clarify this

l.99 : Doesn’t the 1D model need single-scattering albedo ϖ? Would it be more appropriate to introduce first the 1D model (reverse 2.1 and 2.2) to highlight what properties are needed? Maybe consider to make the link between F_{ice} and ϖ as follows (valid for weakly absorbing media):

$F_{ice} = B \cdot \rho/(\rho_{ice}+(B-1)\rho)$, where B is the absorption enhancement parameter (see Libois et al., 2019)
And $1- \varpi = 2B\kappa/(\rho_{ice}\,SSA)$ (Picard et al., 2016)

l.102 : unclear. Should it be the distance between extinction events (which can either be scattering or absorption)? And the relation is simply the inverse, no? Could you use there the more straighforward expression of extinction coefficient as density x SSA / 2 (depending on whether you include diffraction or not in scattering). See for instance Malinka (2014).

l.115 : could you comment on this wavelength dependence. Is it a default of the method, or something expected?

Eq. (4) : typo sign error; also, sin and cos should not be italic (same think throughout the paper)

l.137 : add v_r and v_t in parentheses here, and remove the end of the sentence l.141

l. 142 : this sounds very awkward to mention individual snow grains here, while the advantage of working with X-ray microtomogography images is to get rid of the particular representation of snow. Also, it is obvious that isolating grains from such an image is very arbitrary and isolated grains can behave very differently than the same grains being slightly sintered. Definitely it’s not tricky to define the phase function of a porous medium based on local characterization (see for instance Haussener et al., 2012). This deserves more caution. The approach of Xiong et al. (2015) might be more appropriate than isolating “snow grains”. An illustration of the segmentation process would be useful if this strategy is maintained. Could you also provide (where it best suits) the values of the asymmetry parameters obtained with this approach?

l.170 : this grain selection seems very arbitrary and would deserve more attention or explanations. Also, how many grains should be averaged to have something representative? What’s the variability of the phase function across grains from a same sample?

l.172 : some comment is needed on the relevance of using the properties of a very small sample to represent a whole (necessarily heterogeneous) snowpack. Said differently, what is the representativity of the sample?

l.175 : reference to Picard et al. (2016) might be relevant

l.176 : problem with the beginning of the sentence

l.198 : could you double-check the equation for μ_y. There might be a sign error. Also didn’t you forget the last terms for μ_x and μ_y?

l.202 : is this approach the initiative of the authors, or was it taken from another paper? I’m afraid it’s wrong because it overall underestimates the total distance traveled by a photon (the distance traveled between scattering events does not include enhancement in the ice phase), hence the total absorption. This is probably tricky.

l.207 : the “Russian roulette” should probably be better explained. What happens to the photon packets that are not killed?

Figure 3 : labels should be larger (also for Figs. 9, 10, 13). Why using markers? Why not simply having two layer with different shades?

l.227 : I did not understand “is used to simplify the complex reflectance properties of a rough surface”

l.238 : not clear whether samples are taken from the surface or in the pit (to sample various layers)

l.241 : how later (compared to snow sampling) were the images taken?

l.245 : “optimization” is unclear

l.247 : was it nadir observations?

l.255 : what’s the size of the aluminium panel? How was it practically inserted? How did you ensure that it is horizontal under the snow? What’s the precision of the depth position (transmissivity greatly varies with depth)? 4.75 cm seems very (too) accurate for a depth measurement! Typo for “aluminium”

Figure 4 : maybe not very useful.

Figure 5 : An indicative scale would be helpful

l.271 : Is the cylinder still 7 cm high for the detailed analysis, or limited to a cubic sample?

l.281 : totally agree, and this should be further discussed. Does this literature correspond to optical studies? If not, I see no reason that this approach is satisfying for optical issues.

l.313 : what is the underlying albedo? Visible light can indeed reach the ground

l.317 : “of the each”

l.318 : how is albedo computed? What are the illuminating and viewing angles?

l.320 : “that favors” reads awkward → “it shows the strong sensitivity of NIR albedo to snow microstructure”

l.323 : it’s more a dependence than a relationship

l.325 : is exponential qualitative or confirmed? Consider referring to Eq. 9 of Kokhanovsky and Zege (2004)

Figure 10 : 25000 photons per wavelength (how many by the way?) or for all wavelengths?

l.326 : what “observed” behavior? Your work or from the literature?

l.326 : “with good fidelity” is not justified. What do you compare to? More generally your model could not but reproduce that, so it’s not a proof of the model being “good”.

Table 1 : would be useful to provide the parameter B as well (see Libois et al., 2014). In particular the values would be 1.95 for fine grain and 2.05 for coarse grain (TBC). Also γ_{ext} is quite different from $\rho \cdot SSA/2$ (see Libois et al. 2013 or Picard et al., 2016), which would certainly deserve some comment. Have you applied your technique to a collection of isolated spheres (with known ρ and SSA) to check whether you can obtain the exact (known) value of γ_{ext}?

l.332 : it’s not clear what transmissivity is here. It it the flux at a particular depth within the snow layer of 20 cm? Or it it the transmittance of a snow layer of thickness X (with black surface beneath), where X is varying. Without precision I’d assume it’s option 2. This makes a big difference and should be clarified.

l.336 : an optical thickness is unitless. The penetration depth is a length, though

Figure 12b: shouldn’t the lines be removed, and the red line added to 12a? Because they correspond to transmissivities, not differences in transmissivities

Table 2 : as for Table 1, I found B values ranging from 2.3 to 2.8, which are somehow much larger than previous estimates. Again γ_{ext} is quite different (30%) from $\rho \cdot SSA/2$ (or even $\rho \cdot SSA/4$ if diffraction is not considered). Also, depth seems to start from the ground, which is surprising (looks more like height). Finally, I doubt that SSA estimation can reach 0.01 $m^2\ kg^{-1}$ precision.

l.345 : why not using the 4% reflectance mentioned earlier?

l.347 : I don’t understand what “remarkably good” means, given that substantial differences are seen in Fig. 13. Why are the differences in the NIR so large?

Figure 13 : why is there a line in between points?

l.350 : errors in the phase function are mostly impacting the NIR, but they also affect the visible range, which is why it deserves much more attention.

l.363 : according to the formula presented above ($F_{ice} = B \cdot \rho/(\rho_{ice}+(B-1)\rho)$) it’s no surprise to have a linear-like behavior in the explored range of snow densities. However the 0.25 residual is surprising. I’d be worth computing B for all available data based on your approach.

l.372 : this has been known for a while (Eq. 23 of Bohren and Barkstrom, 1974)

l.368 : again, use the product $\rho \cdot SSA$ instead of a bilinear regression. Again a residual in such regression should be commented.

l.372 : what does a r^2 of 0.25 mean in terms of correlation?

l.380 : suggest → confirm

l.387 : can you clarify what “we pair” means

l.390 : not clear why the highly scattering nature of snow explains the different sensitivities to F_{ice} and γ_{ext}. I’d use an analytical expression of the penetration depth (see for instance Libois et al., 2013) to show that the dependence on γ_{ext} is linear, while the dependence on B is square root (changes in F_{ice} are proportional to changes in B if density is unchanged). The ~3 scaling of γ_{ext} results in a ~3 scaling of penetration depth. The ~2.3 scaling in F_{ice} results in a ~1.5 scaling, which is consistent with your simulations.

l.392 : never exceeds 2.5 cm, no?

l.393 : leading to **an** increase

l.398 : for crust layers, how would you isolate grains from the 3D image?

l.404 : at what wavelength were the phase function and γ_{ext} estimated ?

l.407 : unit missing

l.422 : I don't agree with "high accuracy"

l.425 : at what wavelength?

l.426 : was the reduction of albedo mentioned earlier?

l.428 : again, this is obvious

l.435 : consider reading Hagenmuller et al. (2019)

<u>Additional suggestion</u> :

Here is a procedure to test the validity of the 1D ray-tracing code (although I don't particular believe it does not work):

- Consider an homogenous (horizontally semi-infinite) layer of thickness L, non absorbing
- Illuminate it with diffuse light
- Record the path lengths of escaping (reflected and transmitted) photons
- Check that the average path length equals 2L, **whatever the chosen phase function**
- If it does not work there is an issue somewhere
- See Blanco and Fournier (2003) for more details

<u>References</u>

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