Revision of EGUSPHERE-2024-2583 - RC2

We thank the reviewer for a constructive and encouraging feedback, which helped clarify the method and identify different avenues for future development. We address the different comments below, with our answers highlighted in purple.

Major comments

Major comment 1 – I am a little confused by the necessity of developing/using the machine learning (ML) emulator of RTM. Does the optimising retrieval algorithm only work with the ML emulator? Can the algorithm also work/couple directly with the physics-based RTM e.g., BioSNICAR? Or is it just for the computational efficiency purpose?

Reply: The necessity of developing an ML emulator in the context of this study was indeed a matter of computational efficiency, because applying an optimization algorithm to the original model would have been very slow/resource demanding. Emulating the RTM with a neural network improved the efficiency by 1) accelerating the forward runs prior gradient computation and 2) accelerating the gradient computation by leveraging automatic differentiation via TensorFlow [Jouvet et al., 2021]. The algorithm in its current form therefore requires the model to be written/readable by TensorFlow, and hence cannot be applied directly to BioSNICAR, which is written with more common python libraries such as numpy, that do not enable automatic differentiation.
We have changed section 2.1 to clarify this point:
"The inversion scheme is based on the open source RTM BioSNICAR [Cook et al., 2020], a python translation of the SNICAR model [Flanner et al., 2021]. Directly optimizing BioSNICAR via a gradient-descent algorithm would have been too computationally expensive and hence we built and used a deep learning neural network emulator of the RTM in order to improve the efficiency of the inversion, and notably 1) accelerate the forward runs used in the optimisation algorithm prior the gradient computation and 2) accelerate the gradient computation by leveraging the automatic differentiation framework of TensorFlow. A training dataset of simulations of the original RTM was first generated (section 2.1.1) and used to build the emulator (section 2.1.2), which was then coupled to an optimising algorithm (2.1.3) to invert spectral albedo for surface properties, including the darkening effect of light absorbing particles."

Major comment 2 – The authors made a few key assumptions when creating the training dataset, such as two snow layers, spherical snow grains, only upper layer for LAPs, and constant snow density, which limit the applicability of the emulator. Among these assumptions, the top 2 cm snow layer containing LAPs and constant density are probably two most important limitations, which could be relaxed to allow them to vary during the emulator training to increase the applicability of the emulator for future studies. Particularly, only the top 2 cm containing LAPs is not realistic.

Reply: We agree with the reviewer that a fixed configuration of the RTM in principle limits the applicability of the emulator, but we would argue that there are a number of advantages in proposing a simplified configuration, notably because the number of free parameters as input of the emulator must be balanced with both the available knowledge to constrain these parameters and the simplifications inherent to the physical model. In this study, the choice of parameters results from an extensive manual

testing to understand the sensitivity of the model to each parameter and subsequent identification of an optimal configuration that captures the processes of interest (changes in SSA, LWC, and concentrations of LAPs) whilst reducing the number of free parameters. In the paper, we show that the emulator is able to reproduce the signature of a wide range of surface conditions, and hence we argue that this limited configuration may be helpful for forward modeling experiments to avoid tuning a large number of parameters.
We clarify our reasoning regarding the different parameters fixed in the training dataset below, in particular for the depth and density, and hope that it provides a better justification for the design choices of the study and future avenues for development.

Depth of light absorbing particles We agree with the reviewer that this is a simplification and that the depth of light absorbing particles varies in practice, both during the season and between the types of light absorbing particles, hence enabling the emulator to model LAPs in several layers is an important avenue for future developments. Here we decided to fix it to 2cm because 1) it is the depth commonly reported for snow algal studies, 2) the effect of LAPs below 2cm can be modeled with equivalent concentrations in the upper 2cm layer, 3) the size of the training dataset would have grown too large with additional configurations of BioSNICAR and 4) our main goal in this study was to quantify the impact of LAPs by inversion, which is not affected by the depth at which the LAPs are implemented in the model because the inversion algorithm will simply adapt the retrieved concentration to match the apparent properties of the LAPs. As such, the concentration of LAPs in the emulator must be understood as a "2cm-equivalent", which we clarified in the text: "A 2 cm depth was chosen for the upper layer as this depth was used to quantify algal cells in recent field studies [Engstrom et al., 2022, Healy and Khan, 2023], hence the LAP concentrations represent 2cm-equivalents".

Snow density In SNICAR/BioSNICAR, snow is represented as a collection of grains and the effective size of the grains essentially drives the effect of the snow physical properties on the spectral albedo [Flanner et al., 2021, Wiscombe and Warren, 1980]. The effect of the density on the spectral albedo is in comparison minimal, which is why we decided to fix the snow density to an average value and work solely with the SSA. We have clarified this in the methods:
"The density was kept constant at 600 kg m^{-3}, because it minimally impacts the spectral albedo in comparison to the snow grain size, which is here an effective optical grain size [Gardner and Sharp, 2010, Warren, 1982] that covers realistic ranges of snow specific surface area for melting snow (1-10 m2 kg^{-1}; Dumont et al. [2017], Tuzet et al. [2020])."
We agree with the reviewer that in practice snow density is an important physical variable determining snow albedo, and other physical representations of snow may better account for it [e.g. Malinka, 2023], also offering improvement avenues for the emulator.

Snow layers We agree with the reviewer that snow columns contain many snow layers with varying densities in reality, and here we chose to restrict the configuration to two layers mainly as a matter of computational resources. If we had increased the number of layers while allowing the SSA to change in each layer, the size of the training dataset would basically have become unreasonably large both in terms of storage and RAM to train the emulator. This is even more true if the SSA + the LAPs were to vary in the layers. In contrast, if we had added more layers but fixed the variables in the layers, then the resulting configuration would have been equivalent to the current configuration. A possible computationally-efficient improvement avenue to have more layers would be to parametrise the SSA of the snow column as a function of the SSA of the first layer, and we are hoping to explore this possibility in future work.

Spherical snow grains We agree with the reviewer that this assumption limits the applicability of the emulator, as also pointed out by Reviewer 1. We have now added a paragraph to discuss this issue and mention alternatives:
"Snow grains were represented by spheres as per the original formulation of the SNICAR model [Flanner et al., 2021, Wiscombe and Warren, 1980]. Recent work showed that light penetration in snow is better represented using irregularly shaped grains [e.g. Robledano et al., 2023], notably yielding more accurate retrievals of snow specific surface area (SSA), but here we chose to use spherical grains mainly because 1) one objective of this study was to incorporate liquid water in snow using the validated framework of Donahue et al. [2022], which is based on spherical grains, and 2) the main focus of the study was the retrieval of light absorbing particles rather than snow physical properties, hence spherical-equivalent snow SSA were deemed appropriate. Future developments of the emulator may consider more realistic physical representations of snow such as a collection of hexagonal plates [Whicker et al., 2022], irregularly shaped grains [Picard and Libois, 2024], or a random mixture of ice and air phases characterized by their mean chords [Malinka, 2023]."

Major comment 3 – Does the inversion algorithm search for local optima or global optima? Would there be equifinality issue? Also, how sensitive is the algorithm retrieval result to the initial guess and how to effectively select the initial guess?

Reply: The inversion algorithm is a simple stochastic gradient descent algorithm, and hence it does not particularly search for a global optima. However, the tests conducted in section 3.1.2 show that the algorithm is able to retrieve the optimal solution (global minima) from a simulated spectrum (i.e, the error in the retrieved parameters is negligible) and this was verified for 20 independent pseudo-random intial guesses. The application of the algorithm to ground measurements in section 3.2 then shows that the algorithm retrieves a consistent and quasi-unique solution for a measured spectrum (i.e. negligible variation between the 20 retrievals; line 205-208). Hence, the equifinality and sensitivity to the intial guess do not seem to be an issue in our study, as the algorithm reaches the same optimal solution regardless of the initial guess.

Minor comments

Minor comment 1, line 95: What is the reason for the biosnicar discontinuity around 2.5um?

Reply: We do not know exactly what causes this discontinuity, but known issues exist with for example with the Eddington solver for specific combinations of parameters [Toon et al., 1989], and a similar issue may cause these numerical errors.

Minor comment 2, line 223-250: How did the authors compute the radiative forcing from albedo reduction? What downward solar radiation data did the authors use?

Reply: The downward solar radiation used was directly measured at the local weather station, as described in the methods section 2.3, which has been changed for better clarity:
"The daily and instantaneous radiative forcings (W m^{-2}) were calculated by multiplying the BBA reduction with respectively the 24h daily averaged and instantaneous shortwave incoming radiation, as

measured with a four-component radiometer (CNR4, Kipp and Zonen, The Netherlands) at the local weather station [Pirk et al., 2023]."

Minor comment 3: I would suggest adding a section to discuss uncertainties involved in the ML-based emulator and the inversion algorithm.

Reply: We have dedicated a specific result section to the description of the errors of the neural network in the training and validation (3.1.1) as well as the retrievals of the inversion algorithm on both simulated spectra (3.1.2) and measured spectra (3.1.3), hence we are not sure how to add further discussion on the uncertainties of the emulator and inversion algorithm in the present manuscript.

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