egusphere-2026-510 - Some insights from the second principle of thermodynamics for snowpack modeling
Answer to Referee 1

We thank the referee for their helpful review of our manuscript. Please find our point by point response to the review below. The text of the review is reported in blue with our corresponding response just below. Proposed addition to the manuscript text are given in green.

This research aims to improve numerical stability by incorporating constraints derived from the second law of thermodynamics into the model and by developing an algorithm that prevents violations of physical laws, such as decreases in entropy during numerical calculations. Numerical snowpack models involve complex processes, including phenomena that require fine spatial resolution and others that evolve over short timescales, making it difficult to adopt longer time steps. In this respect, the present study has the potential to improve numerical snowpack models in terms of numerical stability while also reducing computational time.
My suggestion is to include a discussion of computational cost. For example, when the same time step is used, does the use of the Tightly Coupled scheme and the Backword Euler method increase the computational cost? If so, to what extent. This discussion helps to explain the advantage to incorporate these schemes in terms of computational cost.
This study addresses several important processes, including coupling with a canopy model and water vapor transport. I expect that, in the future, the framework can be extended to include liquid water movement as well and be further integrated into a numerical snowpack model.

Numerical cost is indeed an important feature of numerical models and opting for a tightly-coupled framework instead of a sequential coupling tends to result in an increase of the numerical cost. However, (i) with specific designs, the numerical cost increase can be minimized, and (ii) as sequential coupling can require to adjust the timestep to maintain stability, it might ultimately result in a larger numerical cost to run the same simulation, without guarantee of success.

Concerning the snow-canopy model presented in our manuscript, using a sequential coupling consists in a two scalar equations (solving for the canopy and canopy air temperatures, neglecting the non-linearity of the longwave radiations for the argument) and a tri-diagonal $N \times N$ system of equations (solving for the snow temperature, N being the number of snow numerical layers). Using Thomas' algorithm for the tri-diagonal system, the problem can essentially be solved in $O(N)$ operations. The tightly-coupled problem consists in a $(N+2) \times (N+2)$ system of equations, that is not tri-diagonal (due to the three ways connectivity between the snow surface, the canopy, and the canopy air). While Thomas' algorithm cannot be directly applied on such a system, the tri-diagonal block corresponding to the snowpack equations can be eliminated using Schur complements. Specifically, the matrix associated with the system of equations writes:

$$
\left(\begin{array}{cc|cccccc}
\bullet & \bullet & \bullet & & & & & \\
\bullet & \bullet & \bullet & & & & & \\
\hline
\bullet & \bullet & \bullet & \bullet & & & & \\
 & & \bullet & \bullet & \bullet & & & \\
 & & & \ddots & \ddots & \ddots & & \\
 & & & & \ddots & \ddots & \ddots & \\
 & & & & & \bullet & \bullet & \bullet \\
 & & & & & & \bullet & \bullet
\end{array}\right) \tag{1}
$$

where $\bullet$ represents non-zero elements, and where the first row/column stands for the air canopy temperature equation/value, the second ones for the canopy temperature's, and the rest for the snowpack temperatures'.
The bottom block matrix being tri-diagonal, computing its Schur complement can be performed with Thomas' algorithm in $O(N)$ operations, and the overall system simplified to a $2X2$ problem. The overhead associated with the full coupling is therefore modest compared to the sequential scheme and does not blow up with the number of snowpack layers.

Moreover, as mentioned above, the tightly coupled system has the advantage of being able to run with any timestep value. To the contrary, the sequential scheme is quite unstable and requires unpractically large timesteps to have stability. As shown in Fig. 1 below, by adding a soil to our system, we were also able to build a test case where the sequential problem is always unstable whatever the chosen timesteps. Essentially, spatial refinement at the bottom of the snowpack to capture the transition between the snow and the ground requires a small timestep for stability, while the canopy/snow/air coupling requires a large timestep for stability. Both are incompatible and instabilities form either at the top or bottom of the snowpack (or both).

For the vapor model, it is not clear if such simplifications to the numerical cost could be done. Indeed, while a sequential scheme (in the sense that equations are solved one after the other as usually done in snowpack models) could be constructed as two $N \times N$ tri-diagonal matrices, the tighly-coupled scheme consists of a $3N \times 3N$ matrix, that cannot be easily simplified with a Schur complement. Thus, the tightly-coupled scheme would be more significantly expensive, especially for large N. But the trade-off for this higher cost would be some form of unconditional stability, compared to a sequential treatment. If one can ensure that a model never leaves its region of conditional stability, then enforcing strict entropy-production is not necessary (at least from a stability point of view).

We will mention in Sect. 6.3 that entropy-compliant schemes tend to be more computationally costly and there is therefore a trade-off between the associated overhead and the possibility to run the model with arbitrary timesteps and on arbitrary grids:

On one hand, the second principle clearly favors numerical stability, and its compliance in models can only increase their overall robustness, alleviating controls on the timestep or the spatial grid. On the other hand, it appears that respecting the second principle is not directly equivalent with numerical stability. [...] Moreover, as they involve more complex numerical problems, strict entropy-consistent models usually present an overhead cost compared to simpler implementations. In the case of the snowpack/canopy model, the use of Schur complements to couple the subcomponents can strongly mitigate this increased cost (Zhang, 2006). However, such techniques cannot easily be employed for the vapor model of Sect. 5. At the same time, strict entropy-compliance favors the use of relatively large timesteps, without the need to implement adaptive

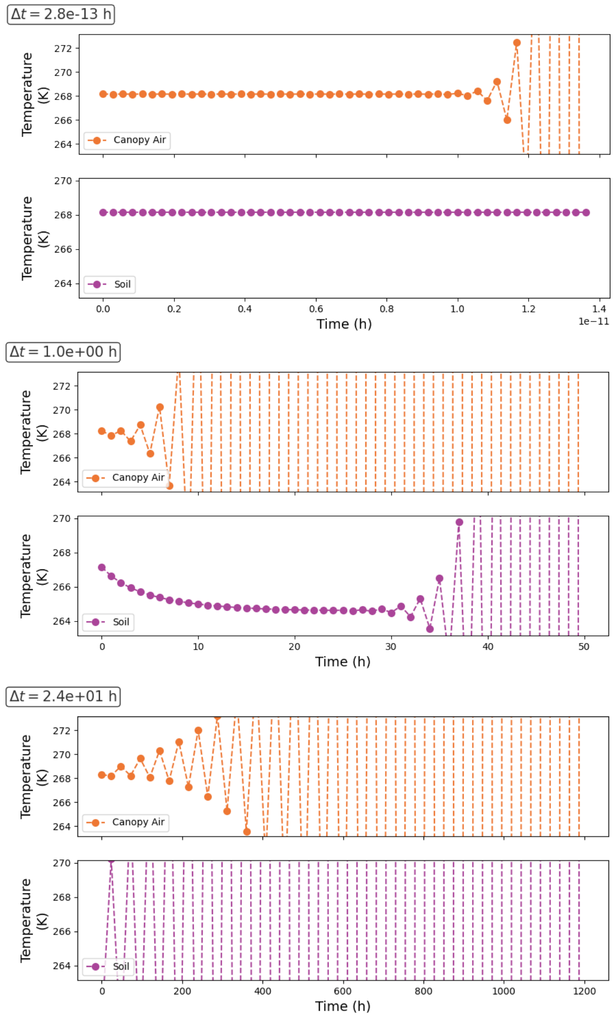

Figure 1: Instabilities developing for every timestep in a soil/snowpack/canopy system with a sequential scheme.

time stepping or rewind strategies. Overall this can result in a significant speed-up compared to less robust models run in their instability regions.

As a consequence, there is a trade-off between the increased stability of entropy-consistent models and their increased computational cost. This might be beneficial in some situations, but not always, depending on the system of equations to be solved and the acceptable constraints on the temporal and spatial resolutions. Thus, we think that the compliance of models to the second principle of thermodynamics should rather be viewed as an overall guide and a tool, rather than a strict rule to adhere to.

L134-135 The oscillation shown in Fig. 1 is problematic for numerical calculations. In contrast, the entropy-based method appears to provide greater numerical stability and relax the time-step constraint, which may contribute to improving numerical snowpack models. It would also be valuable to include a discussion somewhere in the manuscript on how much this method could reduce computational cost

For a given timestep, the use of a fully coupled and fully implicit framework increases the numerical cost compared to less complex schemes (provided that the more simple schemes did not diverge and yielded physical relevant results). But the advantage of unconditionally stable schemes is indeed to relax constraints on timestep and the need to rewind the model in case of numerical problems. This can result in a net simulation speed-up when large timesteps are used.
We will mention this point **L785**:
At the same time, strict entropy-compliance favors the use of relatively large timesteps, without the need to implement adaptive time stepping or rewind strategies. Overall this can result in a significant speed-up compared to less robust models run in their instability regions.

L388-398 Figure 3 compares sequential and tightly-coupled simulations to demonstrate whether oscillations occur. Could the authors provide a version of the figure with the same y-axis scale? If the y-axis scales for temperature and entropy differ between the upper and lower figures, it becomes difficult to judge whether there is a difference between the two cases in initial stage. For example, has entropy reduction and temperature oscillation already started in the initial stage?
We have redone the Figure (see below) using the same axes for the temperatures and entropy source in both panels. Note that this way, the sequential scheme rapidly blows out of the scale. This view also shows that during the first few timesteps the heat fluxes are still well orientated, and the entropy source is positive. Then, the first reversal occurs, associated with an entropy destruction, and the system rapidly blows out with oscillations.

L398- 401 I understand that the thermal inertia of canopy air is very small. However, if the calculation remains unstable no matter how small the time step is because the thermal inertia is set to zero, this may suggest an issue with the calculation setup. I don't think it is necessary to repeat the calculations with non-zero thermal interia included, but it would be better if the authors could comment on the magnitude of the thermal inertia if it is assigned to the canopy air.
We further explore this point by looking at the stability of the system when thermal inertia is added to the canopy air. In order to be able to perform a standard linear stability analysis, we considered the longwave fluxes between the canopy and the snowpack to be linear. With this, the system can be deemed numerically stable when the spectral radius (largest modulus of the eigenvalues) of the matrix formulation of the problem is below unity. As seen in the Fig. 3 below, this analysis shows that adding thermal inertia to the canopy air indeed creates a zone of stability for small timesteps, that is not present in the case of a null thermal inertia. However, there still exists a large region of unstability. The critical timestep and canopy air inertia at which this stability region exists depend on the specificities of the problem (thermal inertias and thermal conductances at play). The fact that stability is only conditional might require to either choose a problematically small/large timestep or to set unrealistically large thermal inertia for the canopy air. Moreover, the problem can be made unstable for any timestep by having a sufficiently fine first layer for the snowpack.

This will be mentioned in the manuscript **L401**:
Consequently, further computations (not shown here) indicate that stability for small timesteps can be obtained by adding thermal inertia to the canopy air. However, this stability remains only conditional and tends to disappear with a very fine spatial grid at the top of the snowpack.

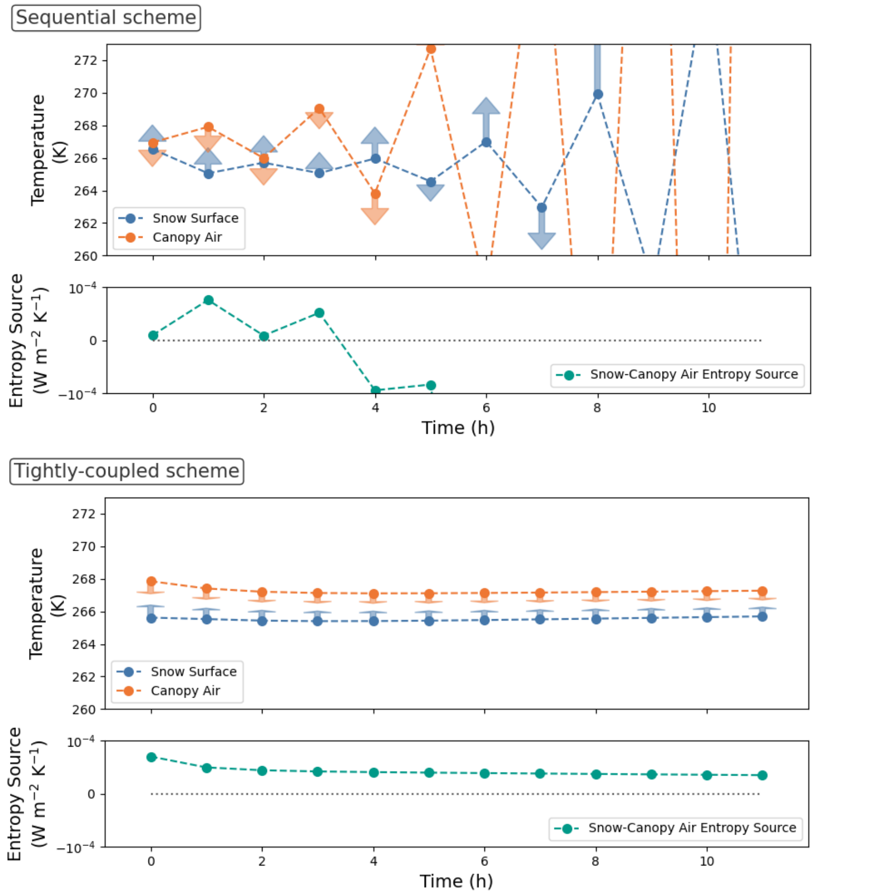

Figure 2: New version of Fig. 3 in the manuscript.

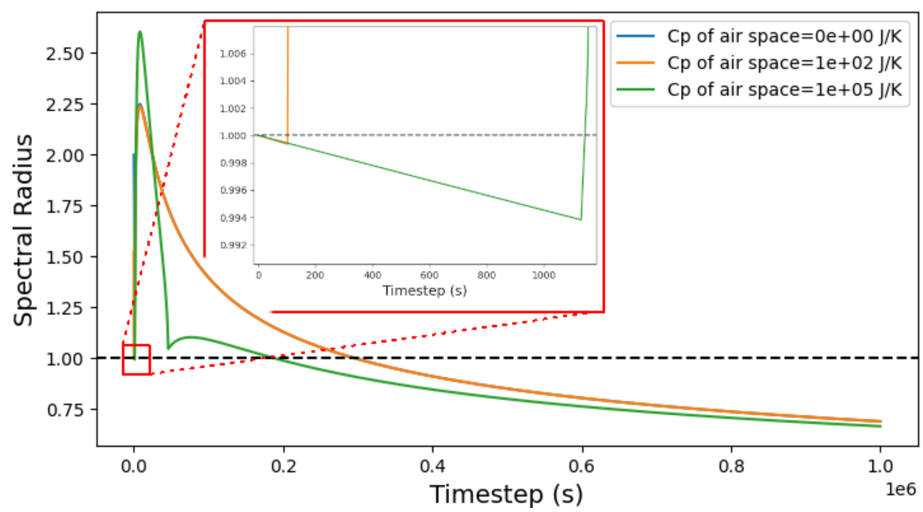

Figure 3: Spectral radius (and stability) of the snowpack/canopy system as a function of timestep and for different canopy air thermal inertia.

L401-403 The fact that the calculations remain stable with very long time steps suggests that it may be possible to calculate changes in external conditions, such as input meteorological data updated hourly, using the same time step. I also wonder whether rapidly varying processes, such as liquid water movement, might likewise be handled with such long time steps. This point may be better discussed in the Discussion section.

The advantage of unconditional stability in indeed to be able to choose the timestep based on the timescale of interest, rather than based on the fastest process at play. In the case of processes occurring rapidly (such water percolation or water refreezing), this allows to maintain a large timestep, and to essentially solve for the equilibrium. Note that as mentioned below in this response, there are also problems associated with the use of iterative algorithms to solve for the non-linear equations involved in liquid water percolation. These methods might fail to find the solutions with large timestep, even said solutions would be stable (i.e. their sequence would not present problems if it were to be found). To the best of our knowledge, the application of entropy-based criteria to design iterative non-linear algorithms has not been fruitful so far.

L497 Is “uv0 and uv0” in Eq. (37) a typo? Should it be “uv0 and sv0”?
Thanks for pointing out this typo. It will be corrected.

L702-703 Are there any actual observations of snow density oscillations on crusts that may be due to similar mechanisms, including findings from previous studies?
To the best of our knowledge, there are no observations of such density oscillations so far. There is indeed the question of whether these oscillations exist but are too difficult to observe, or if they actually do not occur in snowpacks. On one hand, models predict them to occur on a very fine spatial scale, which is not resolved with standard density measurement in the field. Moreover, their formation is hindered by mechanical compaction (Schürholt et al., 2022; Brondex et al., 2023) that tends to smooth out density contrasts. On the other hand, the equations used to model vapor transport in snowpack are homogenized equations that technically only apply at scales orders of magnitude larger than the snow grains. As the density oscillations are centimeter-scale, it remains possible that they fall outside the normal range of applicability of such homogenized model.
In all cases, these oscillations are a fundamental property of the equations governing vapor transport at the snowpack scale (Schürholt et al., 2022) and any models including vapor transport is susceptible of creating such oscillations. It is therefore important to ensure that they do not develop into a physically problematic simulations that might crash a simulation.

We will precise this point **L702**:
We stress that these oscillations are not numerical artifacts, but an actual physical pattern that develops due to the dependence of the vapor diffusivity and thermal conductivity to the ice volume fraction in the model. While to the best of our knowledge such density oscillations have not been observed in the field (either because they are difficult to observe due to their fine structure or because they are hindered by other processes such as compaction for instance), they are constitutive of the non-linear coupled equations used to model vapor transport in snowpacks, and might therefore develop in any model including them. It is therefore important to ensure that they are properly handled by the numerical scheme, and do not lead to problematic behaviors in the simulation.

L711-727 Since this study aims to achieve stable calculations, it is important to summarize how instability can be avoided when a coarse grid provide a new source of instability. The manuscript states that the solution is to use downstream values, but the reason for this solution is unclear. My intuition as a non-specialist is that using downstream values may reduce the amount of heat and water vapor transported, thereby suppressing the oscillation. I therefore wonder whether this is only one specific case in which the using downstream value avoided the oscillation, or whether the using downstream value consistently prevents oscillation across multiple calculation patterns. If it is the former, its usefulness as a general solution may be limited. This point should be discussed more, as it is fundamental to the study’s objective of achieving stable computation.
At the moment, we do not know why the density oscillations occurring with non-linear vapor transport are not bounded and can reach unphysical values for some coarse spatial resolution. At the start of this study

we were expecting the entropy-production criterion to be strict enough to avoid any type of unphysical behavior. The solution of downstreaming was found by trial and error without further justification.
We have performed extra simulations with a different shape for the density crust (square shape instead of Gaussian). As seen in Fig. 4 below, density oscillations form near the crust whose amplitude increases with coarser grids, although we did not reach negative density values in that case. As in the article, these oscillations are severely reduced by using a downstream scheme for the conductivity and diffusivity, suggesting that the downstreaming strategy generally applies for the density oscillations forming near crusts.

A theoretical analysis of this instability would help under their origin and the solution to mitigate them. This is currently investigated by one of the co-author. Since the entropy is degenerated, as pointed out in Appendix B2, there is one direction in the phase space where the evolution is not constrained by the second principle of thermodynamics. Mathematically speaking, the parabolic problem under investigation appears to degenerate, with one hyperbolic direction. For such hyperbolic equations, discontinuities can form in finite time. They have to fulfill what is referred to in the literature as an *entropy inequality*, which encodes the fact that discontinuities should produce some entropies even in this degenerate direction. This translates into an additional condition on the numerical scheme. We refer for instance to Osher (1984) for a simple criterion. Checking the compatibility of our scheme with downstreaming, which is dedicated to a more complex parabolic-hyperbolic system, with Osher's criterion is the purpose of an ongoing study. Note that more classical linear stability analysis cannot be used to explain this problem, as it only appears due to non-linearities.

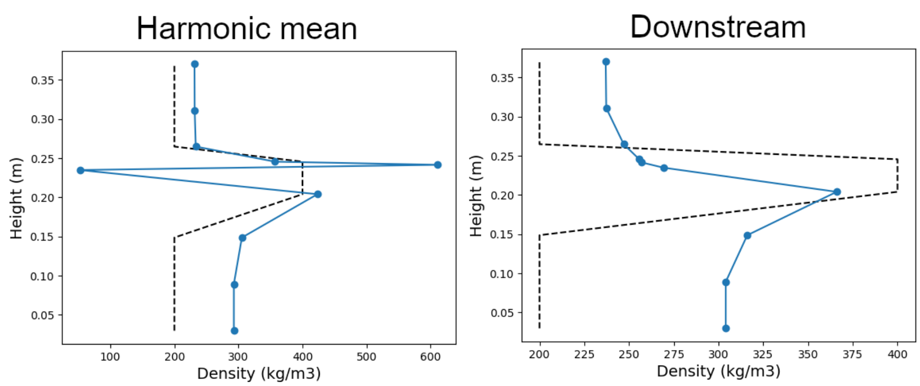

Figure 4: Density oscillation for a square crust without and with downstreaming the transport coefficients.

We propose to specify that the downstreaming strategy appears to apply for different crusts **L720**:
After investigation, we observed through trial and error that a strategy to avoid the occurrence of these artifacts is to use the downstream values for the interfaces' vapor diffusivity and/or thermal conductivity. [...] To ensure that the proposed downstreaming strategy applies more broadly, we performed further simulations with a different crust, this time square-shaped. The results are overall the same. Density oscillations develop near the crust, and they tend to blow out with a coarse grid, although in this case we did not reach negative density values. Downstreaming the thermal conductivity and vapor diffusivity hinder these density oscillations and restore numerical stability.

We will also specify **L685** that the original density crust of the article is Gaussian-shaped.

L730-736 Liquid water infiltration is a major cause of rapid behavior and increased computational cost. If this method can be used to allow larger time steps for such processes, I would expect it to lead to substantial improvement in numerical snowpack models.

We are currently working on describing water percolation and capillary effects in snow with a thermodynamics framework as in this manuscript. However, one of the major difficulty with solving water percolation is the necessity to solve a (strongly) non-linear problem. The sequence of solutions over time (at time n, $n+1$, $n+2$, etc) might be well-defined and stable, but iterative algorithms (such as Picard or Newton algorithms) are not guaranteed to find them and this accounts for a large portion of the numerical cost associated with Richards' equation. We are aware of tentatives to use an entropy criterion to help iterative algorithms converging to the solution, but no clear benefit over other techniques (such as line-searching with a criterion on the residual of the system of equation to be solved) have been demonstrated so far.

The authors of egusphere-2026-510

References

Brondex, J., Fourteau, K., Dumont, M., Hagenmuller, P., Calonne, N., Tuzet, F., and Löwe, H.: A finite-element framework to explore the numerical solution of the coupled problem of heat conduction, water vapor diffusion, and settlement in dry snow (IvoriFEM v0.1.0), Geoscientific Model Development, 16, 7075–7106, https://doi.org/10.5194/gmd-16-7075-2023, 2023.

Osher, S.: Riemann Solvers, the Entropy Condition, and Difference, SIAM J. Numer. Anal., 21, 217–235, https://doi.org/10.1137/0721016, 1984.

Schürholt, K., Kowalski, J., and Löwe, H.: Elements of future snowpack modeling – Part 1: A physical instability arising from the nonlinear coupling of transport and phase changes, The Cryosphere, 16, 903–923, https://doi.org/10.5194/tc-16-903-2022, 2022.

Zhang, F.: The Schur Complement and Its Applications, Springer New York, https://doi.org/10.1007/b105056, 2006.