Three-phase numerical model for subsurface hydrology in permafrost-affected regions
Response to Reviewer #3

Recent years have seen renewed interest in thermal hydrological models of frozen soil dynamics, with the motivation coming from concerns about the vast amount of perennially frozen carbon in the northern permafrost region. Despite significant progress, modeling of active layer dynamics remains a challenging application. Our discussion paper makes significant progress on multiple fronts.

Most significantly, we present the first proof-of-principle simulations of three-dimensional active layer dynamics with appropriate representations of ice-water-vapor partitioning in variably saturated conditions. This capability is being made available to the scientific community in the form of open source software, and we believe it is important make full technical description of the model, validation activities, and the solution method available to the scientific community. The vast majority of previously published modeling results were one-dimensional. We are aware of a very limited number of two-dimensional simulations, but we are not aware of previously published three-dimensional simulations of active layer dynamics. We note that 3-D simulations would have not been possible without high-performance computing because of the computational challenges inherent in the thermal hydrology of freezing soils.

In addition, we simplified a previously published two-component formulation to obtain a thermal Richards equation-based model, in the process illuminating the underpinning assumptions required. We showed, for the first time, that a thermal Richards formulation gives essentially equivalent results to the more complete two-component formulations that allow gas advection. As far as we are aware, all previous models have simply assumed the Richards formulation without consideration of whether the passive-gas approximation is appropriate.

Further, we showed that vapor diffusion, which has almost universally been neglected in permafrost models, may be important in many situations through a subtle and previously unrecognized feedback process in which slow ice accumulations alters the thermal conductivity, and as a consequence, the temperature.

Finally, as has recently been noted by Dall'Amico et al. (2011), previous models used constitutive relations that relate liquid content to temperature that are strictly applicable to gas-free conditions. Our formulation relies on very recently published constitutive relations that are appropriate in variably saturated conditions.

The reviewer suggests that the paper be reshaped with "less clutter induced" by discussion of previous work. We plan to compress the material on Pg 152, which was an unnecessarily detailed summary of previously published work.

We believe further rearrangement would be a disservice to the readership. The paper does indeed build on much previous work by us and other researchers. However, the formulation is new, the constitutive models are only recently available, the numerical implementation in an open-source highly parallel code is the current state of the art, and we have the advances detailed above. It is important to place the contribution in the context of previous work on the subject, and we believe we have a good balance.

We also plan to revise the introduction and the abstract of the manuscript to better clarify the important contributions. In addition, we plan to make a few revisions to the structure of the paper, as described below.

Specific comments:

To aid in following the response, we number the reviewer's specific comments and address them in order.

Comment #1: page 153 line 27- "This paper addresses the details of process representation, and parallel implementation of . . . ": this does not seems to me to correspond to this paper content. Neither the first or the second where detailed, or possibly I and the Authors give a different meaning to the word "details". Actually, detailing the parallel implementation would not be so appropriate in TC, and better suited to a journal about numerics and/or informatics (maybe GMD).
Response: We agree that details on numerical implementation are not of interest here. We will revise the sentence in question to read "… details of process representations and summary of parallel implementation". That revision more accurately represents the content of the paper.

Comment #2: page 154- line 2 - "Use of soil texture information in place of empirical soil freezing curve": where ?
Response: We will revise the manuscript to remove the phrase in question. The calculation of freezing curves from soil water characteristic curves under unfrozen conditions, which may be estimated from soil texture information, was the subject of Painter and Karra, 2014. We will also modify the sentence in question to include model validation, which was not included in the original list.

Comment #3: Equation 1a - The first divergence term contains velocities in different position. Given the commutativity of products, it does not matter. However, symmetry in writing could be better.

Response: This will be fixed in the revised manuscript.

Comment #4: Equation 1b - Soil is explicitly included. However, its role is pretty passive. Understand- ing if the soil matrix is indeed rigid or not is crucial (for understanding if the transition to saturation is well designed).
Response: We will revise the manuscript to make clear that we are assuming a rigid porous medium. We do include compressibility of ice and liquid, and more

importantly compressibility of the pore space. The latter is represented by making the porosity depend on pressure, a standard procedure. We will include this detail in the revised manuscript. We note that this is equivalent to the lumped-parameter approach of including a soil specific storage, but we prefer to have the two terms explicitly written.

Comment #5: Equation 8a-8b - They are crucial for the more relevant results obtained, and should be explained better. Besides, does neglecting non freezing-point depression have consequences on the results ?
Response: We agree that the equations 8a and 8b are critical, but it is not necessary or even appropriate to reproduce detailed work that has already been published. The model in question has been published in Vadose Zone Journal (2014). We will update the citation when we revise the manuscript.

Comment #6: page 158 - Equation 9 is the vanGenuchten parameterisation of the soil water retention curves. Its extension to negative suctions (positive pressures) with a constant could be source of flaws. In this case, in fact, the term containing the partial derivates with time of soil water is null, and water does not move. This term should be extended by using soil specific storage (e.g. Lu and Godt, 2012) to obtain the groundwater equation. Actually, the soil specific storage can be obtained directly from equation 1a. But if it is actually made is not clear in the paper.
Response: We do not include the lumped parameter soil specific storage, but rather decompose it into its physical components: compressibility of liquid, compressibility of ice, and compressibility of the pore space. The latter is, of course, the dominant term. We will revise the manuscript to include that important term, which was in the code but not in the description.

Comment #7: page 163 -line 20 - "The simulations are designed to test whether gas . . . vapour flow". This is the only clear research question I found in the paper related to physics.
Response: We strongly disagree, and we note our general response above.

Comment #8: page 165 - line 12 - I assume that all the parameters vary with water (ice, vapour) contents, according with equation 11. Therefore the parameters' values refer to the small "k" in equation 11. Correct ? It should be clarified. Differently I would be very disappointed.
Response: We agree that thermal conductivity must depend on the phase content. The small "kappa", which is the effective thermal conductivity of the soil, depends on the liquid and ice content according to Eq. 12. Additional dependencies of the saturated and dry thermal conductivities on porosity may be included in an application, but given that little porosity change is expected in any given simulation, such dependence is a matter of model inputs for a site of interest rather than model formulation.

Comment #9: page 162 - Section 6.2 as written is non informative.

Model spin-up, the subject of Section 6.2, is widely recognized in the Earth system modeling community as a key detail in making models work effectively. It is perhaps less widely recognized that it is very important in subsurface modeling work as well. Our experience is that with freezing soil, having an effective spin-up strategy can make the difference between a successful and unsuccessful model. We believe the material in question will be of interest as modelers start to deploy the advanced capability described in the manuscript, but do agree that as written the section is a non sequitur. We plan to move the material in that section to Appendix B. We emphasize that the material in Appendix B is a novel approach to the spinup question that has not been presented before.

Comment #10: page 167 - line 9 - "However, those models have been limited to relatively small scales . . .": In my opinion also this paper sticks with relatively small scale, so the statement is inappropriate, or requires further explanations.
Response: The point is that we have introduced a highly parallel modeling capability that is the enabling technology for doing process-rich simulations at relevant scales. We will revise the text in question to read "... have generally been limited to relatively small scales (e.g. the column scale) and one spatial dimension because of ...". We note that the simulations shown are 3-dimensional and span 25 m in the horizontal and 20 m in the vertical, which is orders of magnitude greater than the column scale. The simulations used 2 million grid cells.

Comment #11: page 167 -line 22 - " However, Mars application . . . will generally require two component model.": this is not an achievement of this paper, so it probably does not belongs to the conclusion of this paper. At least, the concept should be written differently for this context.
Response: This is a "discussion" point. We will change the section title from "Conclusions" to "Discussion and Conclusions".

Comment #12: page 168 - line 11 - "However, the vapor diffusion model .... thus needed". This statement belongs better to a "Discussion" than to a "Conclusion".
Response: See our reply 11.

Comment #13: page 168 - line 14- The statement that starts here can be eliminated. Nobody knows what "high parallel subsurface hydrology" is. This paper is not even on "parallel computing". Maybe is "on the use of a parallel computing infrastructure for simulating sub- surface hydrology": but if this is the topic, I have to say it is not properly treated in the paper. In fact, then I would expect a comparison of performances for instance about how the computing performances by using 1,10,1000 processors, and more discussion about informatics than of freezing soil physics. I also remark, that, if it would be the case TC is not the appropriate outcome.
Response: We will remove the phrase "highly parallel" in the revised manuscript. We discuss the parallel performance on page 161 (lines 1-14) and figure 1.