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> Interactive Comment

Interactive comment on "Estimation of thermal properties of saturated soils using in-situ temperature measurements" *by* D. J. Nicolsky et al.

D. J. Nicolsky et al.

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We are thankful to this reviewer for close reading, and thoughtful suggestions to improve quality of our manuscript. We revised the manuscript according to all issues raised by the referee in the following comments (marked by bold). In a new version of the manuscript, suggestions to specific comments are marked with bold font style.

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Response to the general comments:

Unfortunately the paper is not well organized, which makes it difficult for the reader to follow its logic. Thus the paper should only be published with major revision. The paper should be reorganized in several places to ease following the logic. Section 3 ("Review of existing methods ...") contains parts which (1) typically belong into the introduction, reviewing deficiencies of older methods and motivation for new ones; (2) state the inverse problem (could be merged with Section 6); (3)give an example of the methodology, which could be shortened considerably or omitted. Section 4 ("Solution of the heat equation...") should directly follow the physical setup (Section 2, "Modeling of soil freezing and thawing"). Section 5 ("Selection of an initial approximation") should follow the description of the optimization process (Section 6), because the importance of the initial values depends on the algorithm, as in the case a gradient-type method. It could also be merged with the site-specific Subsection 7.2. Section 5 and Subsection 7.2 are particularly difficult to understand, and should be revised accordingly. Many of the details are probably not important to the reader, while the general idea of constructing physically reasonable subproblems is. The first two paragraphs of Subsection 7.3 ("Global minimization...") would fit perfectly into Section 6.

We agree with the reviewer that the manuscript could be better organized. We closely followed all above suggestions and consequently reorganized the presentation in several places to ease following the logic. Extra special care was taken in Sections 5 and 7.2 of the original manuscript in order to make them clear to understand.

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Response to the specific comments:

1. Section 2: What fluid and ice properties are used?

We use water and ice properties at 0C. The corresponding correction is made in the text.

2. Section 2: Unfrozen water content: As there are many possibilities for the choice of θ_l (see e.g., [Lunardini(1987)] or [Galushkin(1997)]). Why use exactly this function? Is there observational support for this? Is the freezing curve really as 'discontinuous' near 0C?

There are many possible approximations for the unfrozen water content θ_l , with the most common given by a power or exponential functions. We used the approximation, based on the power function, since we had previous positive experience with it. The "discontinuous" function was brought just as an example of possible dependence of the liquid water content on temperature, see [Romanovsky and Osterkamp(2000)] However, in the described approach to find the thermal properties, we used a continuous version, i.e. $\theta_l = (T/T_*)^b$ if $T < T_*$. The corresponding correction is made in the text.

3. Section 2: Boundary conditions: On p. 217, I. 10ff, it is proposed that of Dirichlet boundary conditions (BC) are used at the ground surface and and a depth I. Why choose this kind of BC? In geothermal studies usually a Neumann BC is assumed at the bottom. At which depth I is the BC imposed? On p. 237 an I of 1.06 m is given. Taking the assumed length of time series (t = 120 days / 1e7 s) the thermal depth constant p4 t is a few meters. If this is right, there probably will be numerical problems independent of the type of BC chosen (see, e. g., [Stevens et al.(2007)Stevens, Smerdon, Gonzalez-Rouco, Stieglitz, and Beltrami]). The choice in Fig. 3 is more reasonable. **TCD** 1, S195–S203, 2007

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Several options for boundary conditions at the ground surface and some depth l exist. Namely, the boundary conditions can be of Dirichlet, Neumann, or Robin type. In the geothermal modeling, typically the Neumann boundary conditions are set at the depth l. However, in this article we use measured temperatures at the ground surface and the depth l to set the Dirichlet boundary conditions. The corresponding correction is made in the text.

4. Section 3: The last paragraph is misleading. Some of the results apply only to gradient type methods (which are not used in this article), which are usually meant by "iterative methods". There are many other methods (often of stochastic character), which will not get trapped in the nearest local minimum. Further, non-existence, non-uniqueness, and instability of are common with most inverse problems, in particular data and model are uncertain. Therefore the discussion of uniqueness here is superfluous, as in inverse problems we usually are interested in characterizing a set of possible parameters. Additionally it is not at all clear, how the forcing function (surface temperature) should directly influence the uniqueness condition, if not by complicating the necessary basic physics.

Discussion: Though the idea of solving physics-based subproblems is interesting, the question of its applicability for general situations is open. It would probably not be efficient (or even not work) if the distribution of misfit measures in parameter space do not show elongated or banana-like structures, but bubbly features. The inclusion of more complicated, time-varying physics (e. g., unsaturated soils, fluid flow, salinity) may influence the situation. How would more sophisticated methods like Markov Chain Monte Carlo or Genetic algorithms on the problem (without the subproblem step)?

Identification of thermal properties by exploiting temperature time series is an ill-conditioned inverse problem, which typical has many solutions. In

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[Muzylev(1985)], it was shown that coefficients in the heat equation are uniquely defined if the boundary conditions satisfy several requirements, which are not satisfied in real-life in-situ observations.

There are many methods used to find a minimum of the multivariate functions, including Markov Chain Monte Carlo and Genetic algorithms. In this article, we focus on a gradient type algorithm that uses an initial approximation to start a minimization problem and also to regularize the minimization problem. Therefore, a special care should be taken to choose the initial approximation. Stochastic and heuristic algorithms can possibly avoid the problem of selecting the initial approximation, but a quality control of the recovered soil properties arises. The obtained soil properties due to non-uniqueness could differ from the physically realistic ones several fold. In this article, we focused on the selection of the initial approximation for the gradient type methods, and review of other methods is out of the scope of this work.

5. Conclusions: What is "commonly exploiting data assimilations"? Which data assimilation methods will be used with the estimates obtained with the methods described in this article? It would be interesting which further applications for the method will the possible.

Variational data assimilation technique is commonly used in mechanics Gladwell(1993)]. mathematics Anderson and Thomson(1992). Murio(1993) oceanography Wunsch(1996)]. heat trans-Beck et al. (1985) Beck, Clair, and Blackwell, fer Alifanov(1994). Alifanov et al. (1996) Alifanov, Artyukhin, and Rumyantsev and geology [Duchateau(1996)]. The initial approximation computed in this article will be used to start the gradient type minimization algorithm to find the minimum of the cost function in our consecutive article that is about to be submitted to the Cold Regions Science and Technology Journal.

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Responses to technical corrections:

- 1. P. 215 and References: Moelders, not Molders Corrected.
- 2. P. 231, Eqn. (25): m_{ij} should be m_{ii} ? Also, having the formulae constraining time steps and cell size would ease the understanding.

Corrected. The formula restricting the time step is inserted.

3. P. 230, I. 10ff and Fig. 3: What is TA exactly?. The behavior of the "lumped TA" curve is strange: Is there any explanation why lumping leads to isotherms jumping from node to node? Which t, which parameter b were **used?** TA stands for the temporarily averaged approximation of the latent heat effects. This strange behavior can be explained by the fact that in the temporarily averaged lumped approach the phase change of water mostly occurs at one grid node. Therefore, as the freezing front approaches the thawed node, its temperature is above 0C and slowly decreases. When this node starts to freeze and the active phase change occurs (majority of water freezes), temperature stays near 0C in the region $\pm \Delta x/2$ near this node, where Δx is a size of the grid cell. When the active phase change has occurred, the temperature lowers in this region very fast, and the 0C isotherm swiftly propagates, resulting in the observed "jumps". Therefore, consistent approximation is better, since it does not allow that, if the time step is large enough. The exact values of Δt are unknown, since it is automatically adjusted, and is bounded between 0.01 and 0.5 days. The value of b is -1.0.

4. P. 247: Computers & Geosciences, not Computational Geosciences

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5. P. 249: No capitals in reference Stafford.

Corrected

Thanks you, D. Nicolsky and V. Romanovsky TCD

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