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Estimation of soil thermal properties using in-situ temperature measurements in the active layer and permafrost

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ABSTRACT

A variational data assimilation algorithm is developed to reconstruct thermal properties, porosity, and parametrization of the unfrozen water content for fully saturated soils. The algorithm is tested with simulated synthetic temperatures. The simulations are performed to determine the robustness and sensitivity of algorithm to estimate soil properties from in-situ high resolution-in-time temperature records in the active layer. and once-a-year measurements in a relatively deep borehole. The algorithm is applied to estimate soil properties at several sites along the Dalton Highway. The presented approach is quite general and can be applied to many problems requiring finding an optimal set of soil properties, and uncertainties in found values.

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1. Introduction

The volume and variety of soil temperature data has drastically increased in recent years. These data are typically composed of two types of observations: high-temporal-resolution temperature records at several depths beneath the soil surface, and instantaneous temperature profiles in a borehole, whose depth ranges from 10 to 100 m. In Fg.1, we show an arrangement of sensors recording high-temporal-resolution temperature used to recover soil properties in this article. Recent increase in collection of these temperature data raises the question of how to analyze and utilize them efficiently. One of the important applications of the measured soil temperature is to reconstruct physical properties of soil such as liquid water content and the thermal properties of the ground material. Once the soil properties are known, they can be used to reconstruct soil temperature dynamics in the past and also to predict its future changes.

There are several methods for determining soil moisture content. Conventional Time Domain Reflectometry (Topp et al, 1980) and drying methods are commonly used to estimate water content in homogeneous soils at shallow depths (Boike and Roth, 1997; Yoshikawa et al. 2004). Moreover. accurate measurement of the total water content can be accomplished by thennalization of neutrons and by gamma ray attenuation. but transportation of radioactive equipment into Arctic regions is impracticable (Boike and Roth, 1997). A review of state-of-the-art methods for measuring soil water content can be found in (Gardner, 1986; Topp and Ferre, 2002). However. the above-mentioned well established methods rely on installation of special equipment in the field, or on laboratory experiments, and hence are not applicable for recovering soil water content from various soil temperature records.

Thermal properties can be also measured in the laboratory or in-situ experiments including the Needle Probe (Herzenand Maxwell, 1959). Divided Bar (Birch, 1950), borehole relaxation (Wilhelm. 1990), non-linear fitting (Da-Xin.1986), thermal pulse (Silliman and Neuzil, 1990), and estimation from thermal gradients (Somerton. 1992) methods. Reviews of some of these methods can be found in Beck (1988). Similar to methods measuring water content, the methods for determining thermal properties are not applicable for recovering thermal properties from typical temperature measurements. i.e. temperature records at different depths. Methods that estimate thermal properties from temperature records include the Simple Fourier Methods (Carson,1963), Perturbed Fourier Method (Hurley and Wiltshire, 1993), and Graphical Finite Difference Method (McCaw et al., 1978; Zhang and Osterkamp, 1995; Hinkel. 1997), They estimate coefficients in the heat equation and yield accurate results for the thermal diffusivity (ratio of the thermal conductivity to the heat capacity) only when the phase change of water does not occur.

One alternative capable of estimating both thermal properties and water content of soil is variational assimilation of temperature

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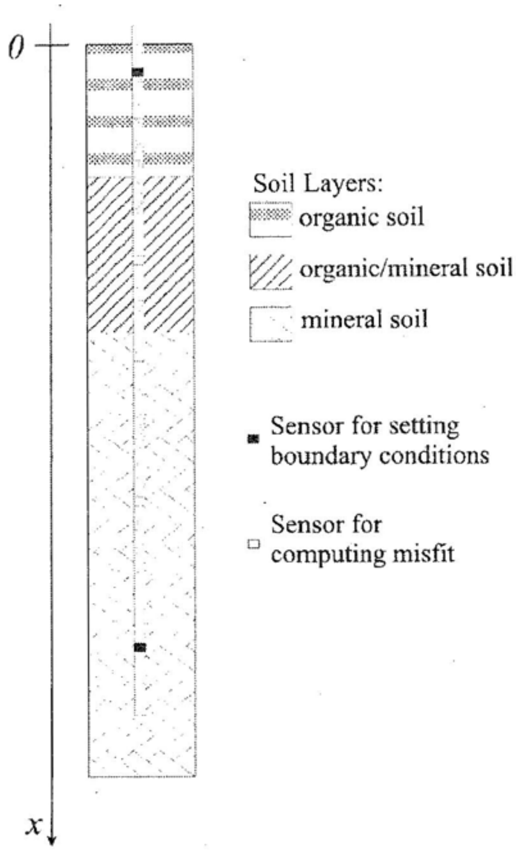

Fig. 1. A schematic arrangement of temperature sensors and a typical geometry of soil layers used in this article to recover properties such as thermal conductivity, soil porosity, and parametrization of the unfrozen water content curve of each soil layer.

observations into a model of soil freezing and thawing. A goal of the variational assimilation is to adjust/optimize a set C of model parameters in order to minimize a difference

$$J(C) \approx \| T_o - T \|^2$$

between the observed To and modeled T temperatures. The set C includes parameters related to thermal conductivity, soil porosity and coefficients determining unfrozen water content for partially frozen soil. Beck (1964) and Nagler (1965) have applied the least square variational approach to estimate thermal properties in a heat conduction problem without phase change. In this article, we compute soil temperature, *T*, by employing the 1-D heat equation with phase change of water (Carslaw and Jaeger. 1959) and minimize the discrepancy *J(C)* by optimizing C.

Numerous books in mechanics (Gladwell. 1993), mathematics (Anderson and Thomson, 1992; Murin, 1993), oceanography (Wunsch, 1996), heat transfer (Beck et al, 1985; Alifanov 1994; Alifanov et al., 1996 and geology (Duchateau, 1996) are devoted to identification of parameters through variational approaches. In addition, Thacker and Long (1988) and Thacker (1989) establish a link between mathematical formulation of the variational data assimilation and statistical formalism. We emphasize that unlike many other methods, the variational approach, when combined with statistical knowledge of errors in temperature measurements, permits the estimation of *a posteriori* errors in the optimized solution (Thacker. 1989).

Results from Beck et al. (1985); Alifanov (1994); and Alifanov et al. (1996) include a detailed mathematical and theoretical analysis of variational temperature assimilation for the heat equation without explicit phase change terms. Some analysis of parameter estimation in heat conduction problems with phase change can be found in Pavlov et al. (1980); Ouyang (1992); and Permyakov (2004). However, it is hard to find discussion of variational assimilation being used to recover soil properties from in-situ temperature measurements in the active layer and permafrost.

In this article, we apply a variational technique to estimate thermal conductivity, porosity, and coefficients describing unfrozen water content at four locations along the Dalton Highway in Alaska. To evaluate the thermal properties, we use daily temperature measurements and a once-a-year temperature profile in 60 m boreholes. Also, we conduct several numerical experiments and explore robustness of recovering the thermal properties. The recovered properties that are associated with the minimum of J(C) are sought by an iterative method. Since there could be several local minima, a thoughtful selection of an initial approximation of C as well as a certain regularization is necessary (Nicolsky et al., 2007). We add to J(C) a regularization that incorporates *a* priori estimate of values in the optimal control *vector.* Besides the regularization, we assume that the soil properties are constants within each soil horizon. This assumption decreases a hundred fold the number of variables in the control *vector* on which the cost function depends, and hence simplifies the problem.

Section-wise the remainder of this article is organized as follows. In Section 2, we describe the model of soil freezing and thawing, provide some details of its numerical realization, and formulate the inverse model. In Section 3, we show the results of twin experiments. In Section 4, we apply the approach to find thermal properties for several locations near the Dalton Highway in Alaska. Finally, in Section 5. we state conclusions.

2. Data assimilation techniques

In this section, we describe key components of the data assimilation technique. The main idea of the data assimilation technique is to optimize the set of model parameters, C. in order to obtain the smallest possible value of J(*C),* where the temperature *T is* computed by the model described in the next subsection.

2.1. Model of soil freezing and thawing

In many practical applications, heat conduction is the dominant mode of energy transfer in a ground material. Within certain assumptions (Andersland and Anderson, 1978; Kudryavtsev, 1978) the soil temperature *T*, (^{0}C) can be simulated by a 1-D heat equation with phase change (Carslaw and Jaeger, 1959):

$$C\frac{\partial}{\partial t}T(x,t) + L\frac{\partial}{\partial t}\theta(T,x) = \frac{\partial}{\partial x}\lambda\frac{\partial}{\partial x}T(x,t), \quad x\in[0,l], \quad t\in[0,\tau]. \qquad (1)$$

The quantities $C = C(T, x)$ [J m^{-3} K^{-1}] and $\lambda = \lambda(T, x)$ [W m^{-1} K^{-1}] represents the volumetric heat capacity and thermal conductivity of soil, respectively; *L* (J m^{-3}) is the volumetric latent heat of fusion of water, and θ is the volumetric water content. The heat Eq. (1) is supplemented by initial temperature distribution $T(x, 0) = T_0(x)$, and boundary conditions at the ground surface $x = 0$ and at the depth *l*. We use the Dirichlet boundary conditions, i.e. $T(0, t) = T_u(t)$, $T(l, t) = T_l(t)$. Here, $T_0(x)$ is the temperature at $x \in [0, l]$ at time $t = 0$; T_u and T_l are *observed* temperatures at the ground surface and at the depth l, respectively.

One of the commonly used measures of liquid water in the freezing soil is the volumetric unfrozen water content (Williams, 1967, Anderson and Morgenstern, 1973; Osterkamp and Romanovsky, 1997; Watanabe and Mizoguchi, 2002). There are many approximations to θ in the fully saturated soil (Lunardini, 1987). Galushkin 1997). The most common approximations are associated with power or exponential functions. Based on our positive experience in Romanovsky and Osterkamp (2000) we parameterize θ by a power function $\theta(T) = a|T - T_*|^{-b}$; $a, b > 0$ or $T < T_* < 0$ °C (Lovell. 1957). The constant T_* is called the freezing point depression. In thawed soils ($T > T_*$), the amount of water in the saturated soil is equal to the soil porosity η. Therefore, we assume that

$$\theta(T,x) = \eta(x)\phi(T,x), \quad \phi(T,x) = \begin{cases} 1, & T \geq T_* \\ |T_*(x)|^{b(x)}|T|^{-b(x)}, & T < T_* \end{cases} \tag{2}$$

where ϕ represents the liquid pore water fraction. For example, small values of b describe the liquid water content in fine-grained soils, whereas large values of b are related to coarse-grained materials in which almost all water freezes at the temperature T_*.

We adopt the parametrization of thermal properties proposed by deVries (1963) and Sass et al. (1971) with some modifications. We express thermal conductivity λ of the soil and its volumetric heat capacity C as

$$C = C_f(1-\phi) + C_t\phi, \quad \lambda = \lambda_f^{1-\phi}\lambda_t^{\phi}, \tag{3}$$

where C_f, and C_t, are the effective volumetric heat capacities, respectively, and λ_f and λ_t are the effective thermal conductivities of soil for frozen and thawed states, respectively. For most soils, seasonal deformation of the soil skeleton is negligible, and hence temporal variations in the total soil porosity, η, for each horizon are insignificant. Therefore, the thawed and frozen thermal conductivities for the fully saturated soil are obtained from

$$\lambda_f = \lambda_s^{1-\eta}\lambda_i^{\eta}, \quad \lambda_t = \lambda_s^{1-\eta}\lambda_l^{\eta}, \tag{4}$$

$$C_f = C_s(1-\eta) + C_i\eta, \quad C_t = C_s(1-\eta) + C_l\eta,$$

where subscripts i, l, and s mark heat capacity and thermal conductivity for ice at 0 °C liquid water at 0 °C and solid soil particles, respectively, Combining formulae in Eq. (4), we derive that

$$\lambda_t = \lambda_f\left[\frac{\lambda_l}{\lambda_i}\right]^{\eta}, \quad C_t = C_f + \eta(C_l - C_i).$$

Hence, the thermal properties λ and C are expressed by only four variables such as λ_f, C_f, η, and ϕ,

Evaporation from the ground surface and from within the upper organic layer can cause partial saturation of upper soil horizons (Hinzman et al., 2001), Therefore, formulae (4) need not hold in the presence of live vegetation and within organic soil layers, and possibly not within organically enriched mineral soil Romaovsky and Osterkamp, 1997), Besides organic and organically enriched mineral soil layers, there are other horizons, all of which can have distinctive physical properties, texture and mineral composition. We assume that there are several horizons, namely: an organic layer, an organically enriched mineral soil layer, and a series of mineral soil layers. We assume that physical and thermal properties do not vary within each horizon, and hence $\lambda_f(x)$, $C_f(x)$, $\eta(x)$, $T_*(x)$, $b(x)$ can be assumed to be constants within each soil horizon:

$$\lambda_f(x) = \lambda_f^{(i)}, \quad C_f(x) = C_f^{(i)}, \quad \eta(x) = \eta^{(i)}, \quad b(x) = b^{(i)}, \quad T_*(x) = T_*^{(i)}, \tag{5}$$

where the index i marks the index of the soil layer. Table 1 shows a typical soil horizon geometry and the commonly occurring ranges for the porosity η, thermal conductivity λ_f and the coefficients b, T_* parameterizing the unfrozen water content.

Table 1
A range of thermal properties for common soil types at the North Slope, Alaska

Layer	Thermal conductivity, λ_f	Porosity, η	b in Eq. (2)	T_* in Eq. (2)
Mineral-organic mixture	[0.7, 1.8]	[0.2, 0.6]	[0.5, 0.8]	[−0.05, −0.01]
Mineral soil(silt)	[1.3, 2.4]	[0.2, 0.4]	[0.5, 0.7]	[−0.1, −0.01]
Mineral soil (gravel)	[2.5, 3.5]	[0.2, 0.4]	[0.5, 0.7]	[−0.1, −0.01]
Mineral soil (shale)	[1.0, 2.0]	[0.1, 0.3]	[0.5, 0.7]	[−0.1, −0.01]

2.2. Inverse *problem*

A starting point in any inverse problem is selection of parameters to be recovered from available data, We note that if phase change effects are negligibly small then the heat capacity C and thermal conductivity λ cannot be resolved separately by analyzing the observed temperature time series; only the thermal diffusivity λ/C can be found (Hinkel, 1997). Therefore, in order to remove ambiguity in determining the soil properties, we set the heat capacity $C_f^{(i)}$ equal to a value that is typical for a soil type in the i-th layer. Consecutively, we define the *control vector* C as a set consisting of thermal conductivity $\lambda_f^{(i)}$, and parameters $\eta^{(i)}$, $T_*^{(i)}$, $b^{(i)}$ describing the unfrozen water content for each soil horizon, or

$$C = \left\{\lambda_f^{(i)}, \eta^{(i)}, T_*^{(i)}, b^{(i)}\right\}_{i=1}^{n}. \tag{6}$$

For each physically realistic control vector C, it is possible to compute temperature dynamics and compare it to the measured data. The available measured data are organized as two vectors: d_a and d_b, associated with high-resolution-in-time temperature records, and once-a-year measurements in the borehole, respectively. In this article, we mark quantities related to the active layer and bore hole measurements by subscripts a and b, respectively. The data are related to the control vector C by

$$\boldsymbol{m}_a(C) - \boldsymbol{d}_a = \boldsymbol{e}_a, \quad \boldsymbol{m}_b(C) - \boldsymbol{d}_b = \boldsymbol{e}_b,$$

where m is the modeled counterparts of the data, and e is the misfit vector. In theory, if there are no sampling errors or model inadequacies, the misfit vector e can be reduced to zero. If there are errors in the data or in the model, the aim is to minimize e by varying the control vector C.

Assuming that the errors e have a Gaussian probability distribution, we define the cost function J according to Beck and Arnold (1977); Tikhonov and Leonov (1996 as

$$J = J_a + J_b + J_r, \tag{7}$$

where J_a, J_b are related to model/data misfit, and J_r is the regularization term:

$$J_\alpha(C) = \frac{1}{2}(\boldsymbol{m}_\alpha(C) - \boldsymbol{d}_\alpha)^t R_\alpha^{-1}(\boldsymbol{m}_\alpha(C) - \boldsymbol{d}_\alpha), \quad \alpha = a, b \tag{8}$$

$$J_r(C) = \frac{1}{2}(C - C_0)^t R_m^{-1}(C - C_0). \tag{9}$$

Here, the superscript t stands for the transposition operator, R_α and R_m are covariance matrices for the data d_α and control vector, respectively. Finally, C_0 is an initial approximation vector containing *a* priori estimates of soil properties based on soil texture, mineral composition and porosity (Nicolsky et al., 2007).

Physically, terms J_a and J_b describe a mean square deviation of the computed soil temperatures from the measured ones, while the term J_r incorporates information about the soil properties that could be derived from the field/laboratory experiments, or from existing soil property databases and published data (Kersten, 1949). Typically, R_m is a diagonal matrix with the expected variances $\{\sigma_m^2\}$ of each control vector variable down the main diagonal. For example, if *a* priori estimates in C_0 are known with large uncertainties, then the expected variances $\{\sigma_m^2\}$ are large, and hence contribution of the term J_r to the cost function J is small. The opposite is also true, Namely, if the initial approximation C_0 is known with a good degree of accuracy, then contribution of J_r is large and a minimum of J is close to the a priori estimates in C_0.

Statistical interpretation of the least square method considers the cost function as an argument of the Gaussian probability distribution (Thacker.1989; Wunsch, 1996) Under this statistical interpretation, the optimal control vector $\hat{C}$ defined by

$$J(\hat{C}) = \min_C J(C)$$

is the most probable combination of the soil properties for the given temperature realization and prior error statistics. To compute the optimal control vector. we calculate the gradient

$$\nabla J = \left\{ \frac{\partial J}{\partial \lambda_T^{(i)}}, \frac{\partial J}{\partial \eta^{(i)}}, \frac{\partial J}{\partial T_*^{(i)}}, \frac{\partial J}{\partial b^{(i)}} \right\}_{i=1}^{n}$$

of the cost function and minimize cost function} by the Quasi-Newton minimization algorithm (Fletcher, 2000). To calculate the gradient ∇J. we construct and solve the so-called adjoint model (Jarny et al., 1991; Marchuk,1995; Wunsch. 1996). The adjoint code is built analytically by transposition of the operator of the tangent linear model. which was obtained by direct differentiation of the forward model code. briefly described in Appendix A.

In order to estimate the thermal properties uniquely. the boundary conditions must satisfy some requirements. i.e. be monotonic functions of time (Muzylev. 1985). In nature. the rapidly changing weather conditions enforce the surface temperature which does not fulfil this necessary requirement. Consequently. the cost function can have several minima due to non-linearities in the heat Eq. (1). Therefore. the iterative minimization algorithm can converge to an improper minimum if the iterations are started from an arbitrary selected initial guess C_g. Nevertheless. with the initial guess C_g within the basin of attraction of the global minimum. the iterative optimization method should converge to the proper minimum even if the model is non-linear (Thacker. 1989). Usually. the initial guess C_g is selected to be in the neighborhood of the initial approximation C_0. Thus. the right choice of the initial approximation C_0 is important for efficient convergence. In (Nicolsky et al., 2007). we provide a detailed step-by-step algorithm to compute the initial approximation C_0.

To obtain physically meaningful results. the covariances matrix R_a has to be defined appropriately as follows. By definition. if all elements in temperature data d_a vector are statistically independent. then R_a is a diagonal matrix with expected variances σ_a^2 of e_a down the main diagonal. Since temperature disturbances at the ground surface decay exponentially with depth. then the soil temperature does not change significantly over hourly time intervals at depths more than 0.10 m (Carslaw and Jager, 1959; Kudryavtsev, 1978; Yershov, 1998). Thus. hourly collected temperature observations are not statistically independent. We note that a typical time scale over which air temperature changes randomly is approximately 10 days (Blackmon et al., 1984). For the Alaska North Slope Region. these air temperature fluctuations can penetrate up to the depth of 0.3-0.5 m and significantly (and randomly) change soil temperature in the upper meter on a monthly time scale. Hence. the covariance matrix R_a is approximately a sparse matrix with some diagonal structures. the sizes of which are equal to the number of temperature measurements collected in one month. For the sake of simplicity. we approximate R_a by a diagonai matrix with σ_a^2, down on a main diagonal multiplied by weights. Each weight is such that the sum of weights corresponding to measurements within each month is equal to one. In our case. we assume that σ_a are equal uncertainties in temperature measurements due to the limited precision of sensors.

Considering a variable ci in the control vector $\hat{C} = \{\hat{C}_i\}_{i=1}^{m}$ as stochastic and non-correlated. it is possible to define errors of the optimally estimated parameters $C = \{c_i\}_{i=1}^{m}$ According to Thacker (1989). the error covariance of the corresponding variables of the control vector can be calculated as diagonal elements of the inverse Hessian matrix H^{-1}. where $H = \{h_{ij}\}_{ij=1}^{m}$, and $h_{ij} = \partial^2 J / \partial c_i \partial c_j$. The most simple method to compute H is to approximate it via finite-differences (Schroter, 1989). Following this approach. we individually perturb the components c_i of the control vector in the vicinity of the optimal values $\hat{C}_i$. After that. the finite-difference approximation of the Hessian can be defined as

$$h_{ij} \approx \frac{1}{2\delta}\left(\nabla_j J\left(\hat{C} + \delta I_i\right) - \nabla_j J\left(\hat{C} - \delta I_i\right)\right).$$

where δ is a positive real-valued number. $I_j = (0, 0,...,1,...,0)$ is an m-dimensional zero-vector whose i-th element is one. and the quantity $\nabla_j J$ represents j-th component of cost function's gradient ∇J. The inverse of the Hessian H can be easily computed since the number m of variables in the control vector C is typically less than a hundred.

3. Twin experiments

The effectiveness of temperature data assimilation in determining soil thermal properties has to be assessed. A convenient methodology. termed the identical twin experiments. has been proposed in meteorology by Bengtsson et al., (1981); Ghil and Malanotte Rizzoh (1991); and Panteleev (2004). We adopt this methodology and apply it to compare true soil properties to their estimated values.

3.1. Identical twin experiment

In the identical twin experiment. we select a control vector C. called the true control vector. and compute the soil temperature dynamics corresponding to it From the computed temperatures. we assemble the true data to $\tilde{d}_a$ imitate observations d_a. Another set of temperature dynamics are then computed using a control vector C that is a perturbed copy of C. We note that temperatures computed for the control C are called the false temperatures. and there is discrepancy between $m_a(C)$ and the true data $\tilde{d}_a$, i.e. $\tilde{e}_a = m_a(C) - \tilde{d} = 0$. Therefore the cost function J(C)(defined by (7-9) in which d_a is substituted by $\tilde{d}_a$) is not equal to zero. The Quasi-Newton optimization scheme is then used to minimize the cost function J(C) and to find the optimal control vector C.

In the identical twin experiment. we observed ground surface temperature T_u near Deadhorse, Alaska to compute the soil temperature dynamics. The modeled ground material has four different layers corresponding to lithology at the Deadhorse site (148°27'W.70°10'N). The layers are organically enriched mineral soil between 0-0.2 m, silt between 0.2-0.9 m, sandy silt between 0.9-2.7 m, and gravel between 2.7-50.0 m, The lower boundary condition T_1 is set by measured temperatures at 50.0m depth. For each soil layer. we select values of parameters in the true control vector C to be equal to the median values of those listed in Table 1. Once the true control is chosen. we compute soil temperature in the upper 50.0 m beneath the soil surface during the period between August 1. 1997 and June 1. 2002. Consecutively. we define the true data d_a as a set of the computed temperature dynamics at depths of 0.15, 0.3, 0.38, 0.46, 0.53, 0.69, 0.84 and 0.99m which are used to measure temperature at the Deadhorse site. Additionally. in the middle of June each year we select from the computed temperatures once-a-year soil temperature profiles (between 5.0 and 50.0 m below the ground surface) to define the true data d_b, To imitate noisy measurements. we add normally distributed white noise (with 0.1 °C standard deviation in upper meter. and with 0.03 °C standard deviation in deep boreholes) to the true data d_a and d_b. Finally. we add noise to the boundary conditions T_u and T_1 used to force the model. These noisy temperature data d_a and d_b and boundary conditions were then used to recover the control vector C by minimizing the cost function J. We note that for the sake of simplicity. the cost function does not have a regularization term J_r in this experiment

We considered an assembly of twenty identical twin experiments. Each of one differs by a realization of the added noise. and the initial guess C_g from which the minimization of J is started. Each twin experiment produces a set $C = \{\lambda_f^{(i)}, \eta^{(i)}, T_*^{(i)}, b^{(i)}\}_{i=1}^4$ of recovered soil perties. Results C from all identical twin experiments are shown in 2. In these plots. recovered soil properties are marked by circles, their true values are marked by crosses. We observe that the soil osity η is found correctly in upper three layers, where active phase nge occurs. Additionally, the results show that it is impossible to mate η for the deep 2.7-50.0 m layer since the ground material d there is constantly frozen. The thermal conductivity is mated correctly for all layers. The quantities b and T_* used to meterize the unfrozen water content θ are found correctly only the second and third layers. One of the explanations for a ificant spread of b and T_* in the first layer is that freezing/thawing urs in the upper layer quite rapidly, and the number of available perature records used for assimilation is not large enough to lve near -0^0C temperature dynamics in the upper layer. In the p 2.7-50.0 m layer, the coefficients band T_* are not found since e is no active phase change at such depths.

We emphasize that in this identical twin experiment, we started all ches in the vicinity of the true control vector, i.e. within ±30% of true values measured entry-wise. Therefore. this experiment ws that the iterative minimization algorithm converges to the per minimum if the initial guess is close to its true value even gh the data were noisy. In real-life experiments where the true rol vector is unknown, knowledge of a good initial guess mmonly equal to the initial approximation) is important.

Fraternal twin *experiment*

In the identical twin experiment, we generated the true data and assimilated it by a model that has exactly the same geometry of soil rs. In nature, the boundaries between soil layers are not strictly ned. and hence locations of these boundaries have some uncertain- Moreover, we assume that the soil properties are constant within layer. whereas in nature they very often "smoothly" vary with h. In this section, we analyze sensitivity of recovery of soil properties respect to the geometry of soil layers by considering the so-called rnal twin experiment (Arnold and Dey, 1986).

Briefly the methodology of the fraternal twin experiment is as ows. The true soil temperature data d_a and d_b are computed by a model in which soil properties λ_f, η, b, and T_* smoothly vary with depth. These true data are then assimilated into a model in which soil properties are constant within each soil layer.

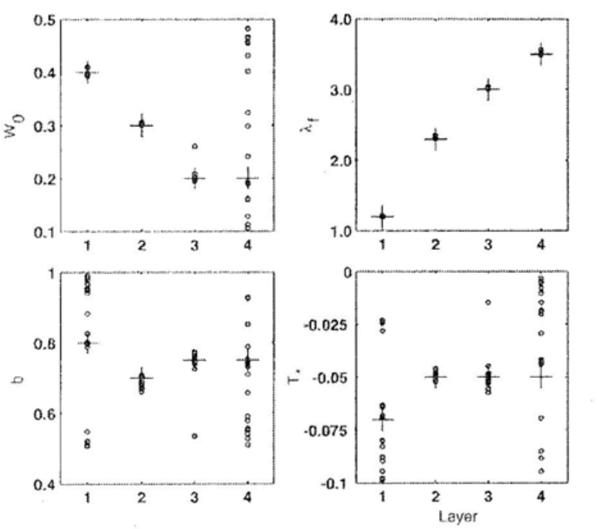

Fig. 2. Recovery of thermal properties and soil porosity for four soil layers in twenty realizations of the twin experiment. Crosses represent true values of parameters being estimated. Circles are estimated values of parameters at the end of each twin experiment.

Before we further consider the fraternal twin experiments. we note that soil temperature records collected in an organic layer cannot be always properly modeled by heat Eq. (1) due to non-heat conductive heat transport (Hinzman et al., 1991; Kane et al., 2001); Romanovsky and Osterkamp, 2001). Therefore. in the fraternal twin experiment. we specify the "surface" boundary condition at some depth. below which non-conductive heat transfer is negligibly small. From the field observation. we know that for Alaskan Coastal plain this depth is 0.2-0.3 m and located at the boundary of the organic/mineral and mineral layer (Romanovsky and Osterkamp, 1997, 2001).

In the fraternal twin experiments, two experiments, A and B, are considered in which we simulate temperature dynamics in ground material located within 0.30-50.0 m below the ground surface. In experiment A, we assume that the ground material is sand-gravel and has higher thermal conductivity comparing to the sand-silt profile specified in B, see the right plots in Fig. 3. Additionally, we assume that the modeled ground materials in both experiments have different soil porosity profiles, shown in the left plots in Fig. 3. In these plots. profiles plotted by smooth lines with stars are used to compute the true soil temperature dynamics. Additionally. we assume that dependence of the unfrozen water content on temperature is the same at any depth, i.e. $\theta = \theta(T)$. But, the unfrozen water content curves $\theta = \theta(T)$ differ between simulations A and B.

In each experiment. after computing the soil temperature dynamics, we add to the temperatures normally distributed white noise, having characteristics as in the identical twin experiment, and then assemble the true data d_a and d_b. We note that the true data d_a is assembled by temperature records at 0.38, 0,46, 0.53. 0.69, 0.84 and 0.99 m depths. The data d_b is defined as in the identical twin experiment, i.e. once-a-year temperature profiles in the middle of June of each year between 5.0 and 50.0 m below the ground surface. The observed temperature dynamics at the Deadhorse site at 0.30 m depth is used to set the upper boundary condition T_u. The lower boundary condition, h is set at 50.0 m depth using the measured temperatures.

Once the true data d_a and d_b are computed. we assume that the modeled ground material has several soil layers (increasing with depth thicknesses) between 0.30 and 50.0 m such that soil properties are constants within each layer. The goal of this experiment is to recover soil properties of each layer based on d_a and d_b. However. analyzing results of the identical twin experiment, we recognize that it is impossible to recover soil porosity and the parametrization of the unfrozen water content for deep soil layers which are always frozen. Hence, we try to recover two numbers: the first one is associated with the soil porosity of the first layer, and the second one approximates the soil porosity of all other layers. We recover two constants approximating b and T_* for all layers (dependence of the unfrozen water content on temperature is assumed to be independent on depth). Also, we find a constant for each soil layer such that these constants approximate smoothly varying thermal conductivity.

Based on knowledge regarding soil texture and mineral composition of the modeled soil, we compose the initial approximation C_0 for experiments A and B. Value of parameters in the initial approximation C_0 for each layer is selected based on its texture listed in Table 1.

As in the identical twin experiment, we investigate dependence of recovered soil properties on the initial guess C_g that is chosen within ± 30% of the initial approximation C_0. We completed twenty fraternal twin experiments and plotted the recovered thermal conductivities and soil porosities in Fig. 3 by step-wise functions. where each "step" is associated with a soil horizon. These experiments reveal that the recovered soil properties are averaged values of the soil properties used to calculate the true data. Instead of plotting recovered values of band T_*, we plot dependence of the unfrozen water content on

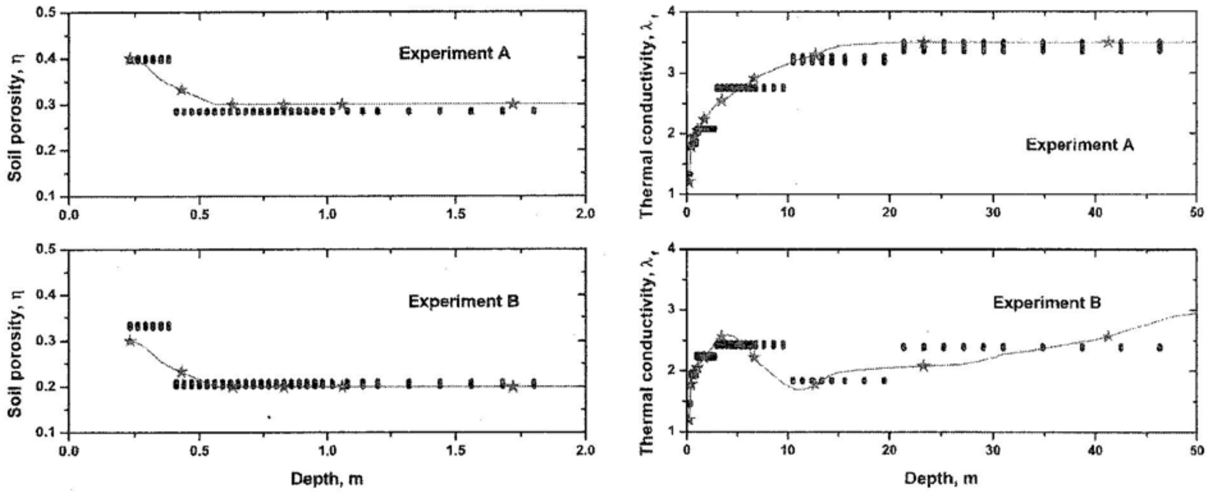

Fig. 3. Recovery of "smoothly varying" soil porosity (left) and thermal conductivity (right) in twenty realizations of the fraternal twin experiment. Red lines with stars represent true values of parameters that are being estimated. The black dots are recovered values under the assumption that the soil properties are constants within each soil layer. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

temperature. The recovered dependence closely matches the one used to compute the true temperature data, see Fig. 4.

4. Reconstruction of thermal properties for sites along the Dalton Highway

To illustrate how the developed technique could be used for specific applications, we apply it to recover soil properties at four sites on the coastal plain of the Alaska Arctic adjacent to the Beaufort Sea. The sites are located along the Dalton Highway and include West Dock (148°33'W, 70°22'N), Deadhorse (148°20'W, 70°10'N), Franklin Bluffs (148°43'W, 69°39'N) and lmnaviat Creek sites(149°20'W, 68°3'N). The soil temperature data were obtained from 1996 to 2007 with sensors measuring hourly temperature at several depths within an active layer and upper permafrost with 0.05 °C uncertainty. The temperature data also include annually measured temperatures (with 0.02 °C uncertainty) in 60.0 m boreholes located at the same sites. Detailed descriptions of site conditions, methods of measurements and data processing have been published in (Romanovsky and Osterkamp, 1995) for all sites except for the Imnaviat Creek site.

Temperature measurements inside a deep borehole are conducted by lowering a temperature probe into a small diameter pipe filled with a convection preventive fluid. Due to minor ground surface disturbance and presence of a metal pipe, temperature measurements in the upper 5.0 m below the ground surface can be biased. Uncertainty in temperature measurements between 5.0 and 10.0 m is 0.03 °C and lower than 10.0 m the uncertainty is 0.02 °C or less.

4.1. Imnaviat Creek site

The temperature sensors were installed on August 26, 2006 at depths 3.0, 5.0, 7.0, 10.0, 15.0, 20.0, 30.0,40.0, 50.0, and 60.0 m, and hourly temperature measurements were taken through June 25, 2007. Since, only 1 year of temperature dynamics is available for this site to assimilate, and since temperature change below 30.0 m is less than uncertainty of measurements, we can assimilate data only between 5.0 and 30.0 m. Therefore, we set upper and lower boundary conditions: $T_u(t)$ and $T_{(1)}$ (t) at 3.0 and 40.0 m, respectively. During the drilling of this borehole, it was observed that the ground material is primarily ice with a small number of boulders, and hence we assume that it can be modeled by a single layer.

At the depth of 3.0 m and below, the ground material is constantly frozen. Therefore, based on results from the sensitivity analysis in Section 2, we can not estimate soil porosity and parametrization of unfrozen water uniquely. We assume that the soil porosity l/=0.90, and the unfrozen water content decreases sharply at T_*,=0.01 °C, i.e. $b=5$. We applied the data assimilation technique and obtained

$$\lambda_f = 2.64 \pm 0.06.$$

The difference between the modeled and observed temperature time series is less than 0.06 °C, Note that thermal conductivity. At for pure ice at -5 °C is 2.2 (Lide, 1999, and the inclusion of small boulders can increase this value.

4.2. West Deck, Deadhorse and Franklin Bluffs sites

Temperature sensors were placed at 0.30, 0.38, 0.46, 0.53, 0.69, 0.84, and 0.99 m depths at the Deadhorse and Franklin Bluffs sites, and at 0.30,0.37,0.52,0.68 and 0.83 m depths at the West Dock site. At these depths, in, this analysis, hourly temperature measurements were used during the following time intervals: at West Dock between August 7.1999 and August 18, 2002, at Deadhorse between July 8, 1997

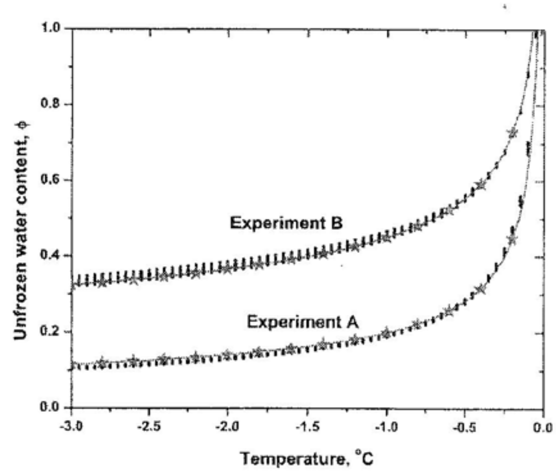

Fig. 4. Recovery of the unfrozen water content parametrization in twenty realizations of A and B types of fraternal twin experiment. Lines with stars represent the true parametrization of unfrozen water content in each type of the experiment. Dotted lines present the recovered unfrozen water content curve at the end of each twin experiment.

Table 2
Thermal properties of the ground material estimated from the best fit of the numerical model to the data

Depth	Soil type	λ_f	η	b	T_*
West Dock site					
0.3–1.0	Silt	1.86±0.01	0.34±0.01	0.75±0.01	-0.045±0.001
1.0–8.5	Silt/sand/gravel	3.21±0.03	0.14±∞		
8.5–50.0	Gravel/sand	3.57±0.05			
Deadhorse site					
0.3–1.0	Silt/sand	2.37±0.01	0.38±0.01	0.61±0.01	-0.045±0.001
1.0–2.7	Sand/silt	3.27±0.04	0.11±∞		
2.7–27.0	Gravel	3.84±0.03			
27.0–50.0	Sand/gravel	3.50±0.06			
Franklin Bluffs site					
0.3–1.2	Silt	2.03±0.01	0.32±0.01	0.56±0.01	-0.029±0.001
1.2–14.0	Gravel	3.64±0.03	0.14±∞		
14.0–17.0	Silt	1.04±0.04			
17.0–21.0	Shale	0.90±0.05			
21.0–50.0	Silt/shale	1.03±0.05			

and June 2, 2002, and at Franklin Bluffs between july 2, 1998 and September 2, 2004. Drilling records were used to determine lithology, see Table 2. Results of previous investigations (Lachenbruch et al., 1982; Lachenbruch and Marshall, 1986; Zhang, 1993; Osterkamp and Romanovsky, 1996) were used to determine the initial approximation C_o. After applying the variational approach, we list the estimated soil properties in the active layer and upper permafrost in Table 2 and compare them to the corresponding values in C_o. We note that the first layer, at the West Docksite, we obtained a good correlation with previous results reported by Romanovsky and Osterkamp (1997), whereas for the first layer at the Deadhorse and Franklin Bluffs sites our estimated values of $\lambda_f^{(1)}$ are higher than the previously reported by 10%, and 20%, respectively. Also we note that for the West Dock and Deadhorse sites, we obtain relatively high thermal conductivities λ_f for the deeper soil layers, see Table 1. These values of λ_f are 10% higher than previous estimates in (Osterkamp and Romanovsky, 1996). We note that for the deep layers between 17.0 and 50.0 m at the Franklin Bluffs, the ground material is a mixture of shale and silt. Usually, the thermal conductivity of shale is lower than the one corresponding for gravel which is widely distributed at the Deadhorse and West Dock sites. Hence we obtain lower values of the thermal conductivity at the Franklin Bluffs site. Our obtained optimal values of the thermal conductivities are 25% lower than the ones given in (Osterkamp and Romanovsky. 1996), but still in the range of commonly occurring values (Andersland and Anderson, 1978). The soil porosity estimated by our approach is within a range of its typical variability (Romanovsky and Osterkamp, 1997).

Using the estimated properties, soil temperature dynamics are calculated for the entire period of measurements involved in this analysis. Results are shown in the left plot of Fig. 5. In this plot. we compare the calculated and measured permafrost temperatures at depths of 0.52 and 0.68 m. In the right plot of Fig, 5, we display a histogram of differences between the measured and computed optimal temperature dynamics at 0.52 and 0.68 m. The mean value of the differences is about 0.01 °C, and their standard deviations are less than 0.08 °C In the left plot of Fig. 6, we show measured and calculated optimal permafrost temperature profiles at the West Dock site on July 3, 1998, June 16, 1999, June 14, 2000, and on June 18, 2001. The largest deviation of the computed temperature from the measured one is a few tenths of a degree in the upper 10.0 m below the soil surface, due to coarsely discretized soil lithology. In the right plot of Fig. 6, we show computed and measured permafrost temperature profiles at the Franklin Bluffs. At this site the thermal conductivity of the deep soil layer is smaller, so the permafrost warming is at much slower rate than at Deadhorse and West Dock, see Fig. 6.

Based on the above examples, we showed the applied variational approach robustly estimates soil properties for various soil types. However, some limitations exist and they are discussed in the next section.

5. Discussion and conclusions

We applied a data assimilation technique to determine soil porosity, thermal conductivity, and parametrization of the unfrozen water content of the active layer and permafrost. Data assimilation permits recovery of these soil proper ties in layers, for which no direct and continuous temperature measurements are available. However, in each case sensitivity of the recovered parameters on the available data has to be analyzed. Based on the results of the performed sensitivity analysis for a typical configuration of soil layer and in-situ observations (the high-temporal-resolution temperature records at several depths below the soil surface, and occasional measurements in a adjacent deep borehole) we conclude that it is possible to estimate thermal conductivity for all soil layers. However, soil porosity and parametrization of the unfrozen water content can be identified only for intermediate layers where active phase change occurs. For other

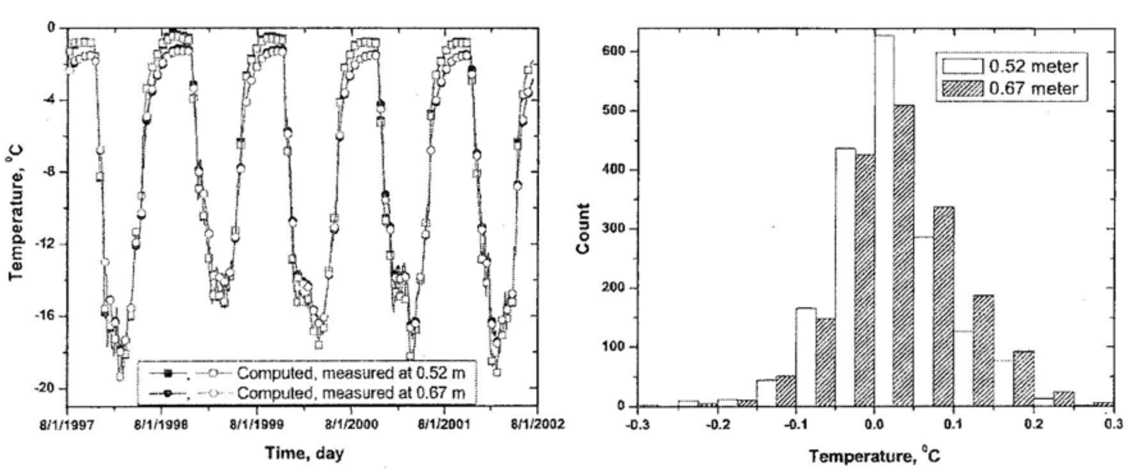

Fig. 5. On the left plot, measured (red) and optimally computed (black) soil temperature dynamics at 0.52 and 0.67 m depth at the West Dock site. On the right plot, the histogram of differences between the measured and computed temperature dynamics shown on the left plot.

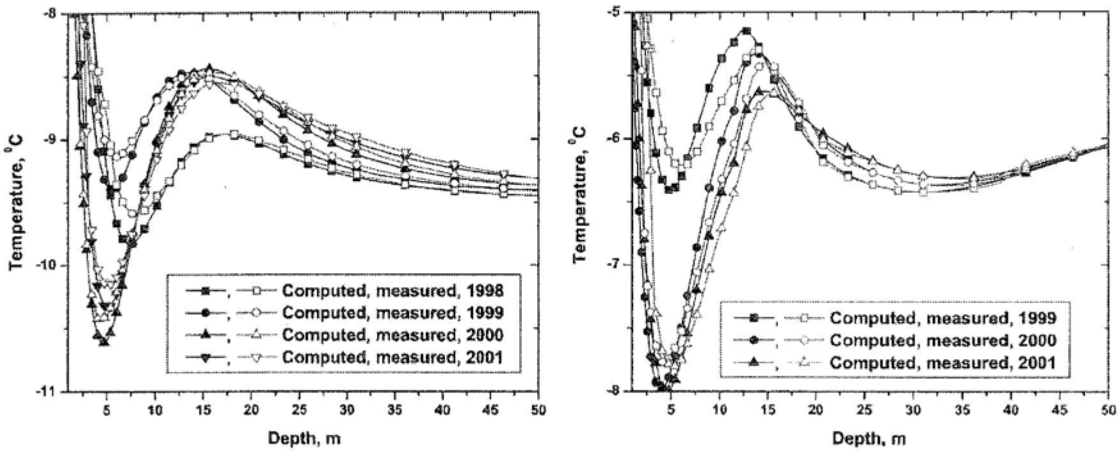

Fig. 6. Measured (red hollow symbols) and computed (black filled symbols) soil temperature profiles at bore holes at the West Dock (left) and Franklin Bluffs site (right) during several consecutive years.

combinations of soil layers and ground surface conditions, additional sensitivity analysis has to be performed in order to establish a set of recoverable parameters.

To regularize *recovery* of soil properties, we incorporate an initial approximation to the soil properties into the cost function. The initial approximation can be found by using available data set (Kersten, 1949), previous investigations, or an approach proposed in (Nicolsky el al.. 2007). In this work, a series of simpler subproblems is *solved* to find C_o and to find a range of variables in C.

One limitation of the variational approach that was used in this work is that it requires certain values of heat capacities in order to find a unique *value* of the thermal conductivity and soil porosity. Also, the applied approach computes the volumetric content of water which changes its phase during freezing or thawing. Water content of liquid water that is tightly bound to soil particles and is not changing its phase can not be estimated within the proposed model (1). Additionally, we used 1-D assumption regarding the heat diffusion in the *active* layer, which sometimes is not applicable due to hummocky terrain in the Arctic tundra. Another assumption used in the model is that the frost *heave* and thaw settlement is negligibly small and there is no ice lens formation in the ground during freezing. Therefore, the proposed method could be only applied where these assumption are satisfied.

Although there are several limitations to the presented approach, we applied it to find soil properties for the West Dock, Deadhorse, Franklin Bluffs and Imnaviat Creek sites along the Dalton Highway in Alaska. The difference between the assimilated and measured temperature dynamics is typically less than 0.3 °C and it is mostly due to oversimplified lithology and physics of soil freezing and thawing. The presented algorithm provided the most probable estimates of the soil properties. The ability to estimate errors in the calculated soil properties is an attractive feature of our algorithm and may be taken advantage of in practice.

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Appendix A. Numerical model of soil freezing

Following finite element framework (Zieniwicz and Taylor. 1991), we approximate

$$T(x,\tau) \approx \sum_{i=1}^{n} \psi_i(x) t_i(\tau).$$

where $t_i(T)$ is a "value" of temperature at the i-th finite element grid, and ?$_i$ is the so-called basis function. After some standard manipulations we *derive* a system of differential equations

$$M(t)\frac{d}{d\tau}t(\tau) = -K(t)t(\tau), \quad t = t(\tau) \tag{10}$$

where $t(T)=(t_i(T))_{i=1}^{n}$ is the *vector* consisting of temperature *values,* $M(t)=(m_{ij}(t))_{ij=1}^{n}$ and $K(t)=\{K_{ij}(t)\}_{ij=1}^{n}$ are the $n \times n$ capacitance and stiffness matrices, respectively. A further refinement, which is often used in finite element modeling of phase change problems, is to exploit a so-called "lumped" formulation, i.e. the capacitance matrix M is diagonal:

$$m_{ij}(t) = \delta_{ij} c_i(t) \int_0^l \psi_i \mathrm{d}x. \quad c_i(t) \approx C(t_i, x_i) + L\frac{\mathrm{d}\theta}{\mathrm{d}T}(t_i). \tag{11}$$

where ?$_{ij}$ is one if $i=j$, or zero otherwise. Dalhuijenson and Segal (1986) provides justification for the lumped formulation on noting that it is computationally advantageous and avoids oscillations in numerical solutions when used in conjunction with the backward Euler scheme:

$$\begin{aligned} \left[M^{(k)} + \mathrm{d}\tau_k K^{(k)}\right] t^{(k)} &= M^{(k)} t^{(k-1)}, & k > 1 \\ t^{(k)} &= t_0, & k = 0. \end{aligned} \tag{12}$$

The main difficulty in numerical modeling of soil freezing/thawing is in consistent calculation of the derivative $d(\cdot)/dT$ in Eq. (11) where $(\cdot)(T)$ is not a continuously differentiable function defined by Eq. (2). In many reviews it is proposed to employ the *enthalpy temporal averaging* to calculate $c_i(t)$. We suggest an approach that incorporates ideas of temporal averaging just to *evaluate* the rapidly changing $(\cdot)(T)$ by defining c_i as

$$c_i\left(t^{(k)}\right) = C\left(t_i^{(k)}, x_i\right) + L\frac{\theta_r\left(t_i^{(k)}\right) - \theta_r\left(t_i^{(k-1)}\right)}{t^{(k)} - t^{(k-1)}}. \tag{13}$$

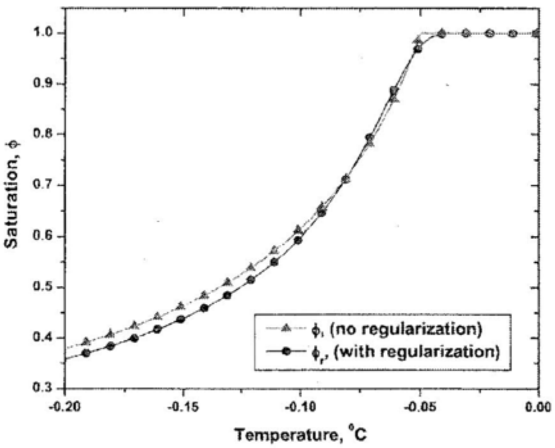

Fig. 7. Dependence of non-regularized (triangles) ϕ and regularized (circles) ϕ_r saturation on temperature.

We note that an advantage of this definition is that it does not compute temporal averaging of the heat capacity and hence reduces numerical computations, and at the same time preserves numerical accuracy of the original idea. Even though that we avoid direct computation of the derivative $d\theta/dT$ by replacing it by the finite-difference in Eq. (13), the calculation of $d\theta/dT$ is still necessary to obtain a solution of the so-called adjoint model used to construct the gradient of the cost function.

We emphasize again that $\theta(T)$ is not a continuously differentiable function, and hence some regularization of θ is required to avoid lost of accuracy in solving the adjoint problem. We propose the following regularization of the unfrozen water content $\theta(T)$ in Eq. (2):

$$\theta_r(T) = \eta|T_*|^b|r(T)|^{-b}, \quad r(T) = T_* + \begin{cases} (T-T_*)e^{-\alpha(T-T_*)^2} & T<T_* \\ 0 & T\geq T_* \end{cases},$$

where if $\alpha\to 0$ then $r(T)\to \min(T, T_*)$ and hence $\theta_r(T)\to\theta(T)$, see Fig. 7. Here, $r(T)$ is an infinitely differentiable function and consequently θ_r posses the same property. One of the advantages of this is that we increase a convergence rate of solving the non-linear heat Eq. (12) by Richardson iterations, precisely find a solution to the adjoint problem, and hence find the location of the global minimum faster than without regularization.

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