Discussion of: "A simple thaw-freeze algorithm for a multi-layered soil using the Stefan equation by Xie and Gough, 2013"

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Abstract

Xie and Gough (2013) developed an algorithm to expand the application of the classic Stefan equation to allow for the prediction of the freeze or thaw depth in multi-layered soils. This discussion paper demonstrates that the development of this algorithm is premised on mathematical expressions that are not physically tenable. A previously proposed equation for applying the Stefan approach to multi-layered soils is herein derived from first principles using the appropriate governing equations, boundary conditions, and initial conditions. Numerical methods are employed to demonstrate the accuracy of this equation derived from first principles. This approach can be implemented in existing cold regions hydrology models to estimate the active layer thickness in permafrost regions underlain by layered soils.

1. Introduction

The classic Stefan equation (1891) has been frequently applied as a parsimonious approach for predicting the active layer thickness (thaw depth) in permafrost or the frost depth in seasonally freezing soils (Jumikis, 1977; Williams and Smith, 1989; Woo, 2012). The active layer thickness and frost depth are important considerations for geotechnical engineers, geocryologists, and permafrost hydrologists due to the hydraulic impedance of pore ice (Kurylyk and Watanabe, 2013; Woo, 2012), the difference in strength properties between frozen and unfrozen soil (Jumikis, 1977), and heaving phenomena associated with freezing soils (Andersland and Ladanyi, 1994; Rempel, 2012).

The governing equations underlying the Stefan approach invoke many simplifying assumptions, including those listed below, that may limit the fidelity of this approach to physical processes (Kurylyk *et al*., 2014a), and thus many variants have been proposed (e.g., Zhang *et al*., 2008). Firstly, the simplest Stefan equation is premised on the assumption that the temperature distribution in the upper thawed or frozen zone is linear, which implies that conduction dominates and quasi-steady-state conditions have been achieved. Secondly, the Stefan equation assumes temporally invariant thermal properties in the upper thawed or frozen zones, whereas the thawed zone may be characterized by pronounced temporal variability in soil moisture and thermal properties (e.g., Hayashi *et al*., 2007). Thirdly, the classic Stefan equation for soil freeze-thaw does not account for heat conduction below the freezing or thawing front, and thus assumes uniform temperatures at the freezing point (0°C) in the lower zone. Finally, the Stefan equation assumes that the soil is homogeneous both with respect to the thermal conductivity as well as the latent heat required to freeze or thaw a unit depth of soil. Several attempts have been made to address this latter limitation by modifying the Stefan equation to accommodate freeze-thaw in layered soils (e.g., Aldrich and Paynter, 1953; Nixon and McRoberts, 1973; Xie and Gough, 2013), and I wish to briefly address the differences in these formulations.

2. The Xie and Gough (2013) algorithm

In their interesting paper, Xie and Gough (2013) provide an approach for predicting the depth of freezing or thawing in multi-layered soils. Herein, the discussion is constrained to soil *thawing* with only two layers to simplify comparisons between approaches. Except where it is decidedly inconvenient, I employ the same nomenclature as Xie and Gough (2013). The simple form of the Stefan equation for predicting the depth of thaw in homogeneous soils is (Jumikis, 1977):

$$\xi = \sqrt{\frac{2k\,I_t}{L\omega\rho}} \tag{1}$$

where ξ is the depth of soil thaw (m), k is the thermal conductivity of the soil (W m^{-1}°C^{-1}), I_t is the total surface thawing index (temporal integral of positive surface temperature since initiation of thawing, °C s), L is the latent heat of fusion of bulk water (334, 000 J kg^{-1}), ω is the mass of pore ice in the initially frozen soil divided by the mass of dry soil, and ρ is the dry bulk density of the soil (kg m^{-3}). Sometimes the right hand side of Eq. (1) is multiplied by a correction factor to account for the volumetric heat capacity of the soil. This form is known as the modified Berggren formula (Aldrich and Paynter, 1953). Note that the product of ω and ρ is equal to the product of the pore ice density and the volumetric pore ice content (volume of ice divided by the total volume of soil), and thus hydrologists who prefer this nomenclature may make these substitutions in any of the following equations.

Xie and Gough (2013) correctly note that two soils with different thermal properties and different moisture contents would experience a different thawing depth if exposed to the same thawing index. Hence they propose the following dimensionless term based on Eq. (1):

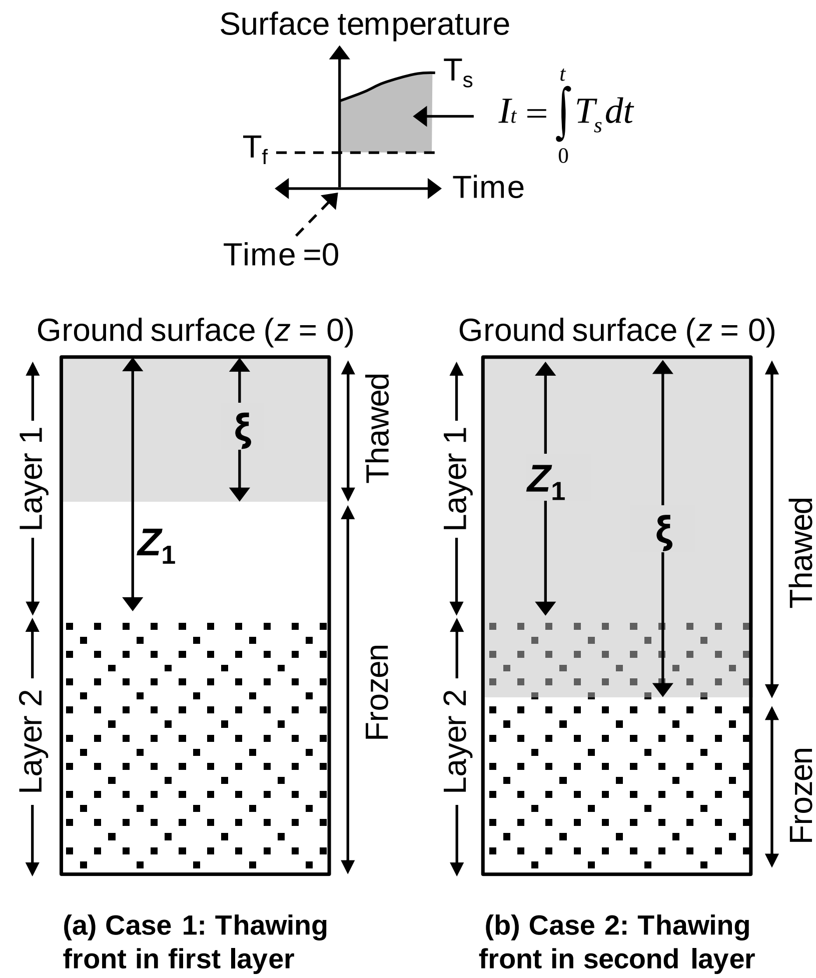

Figure 1: Soil thaw penetration into a two layered soil for (a) when the thawing front is within the first layer and (b) when the thawing front penetrates past the layer interface.

$$P_{12} = \sqrt{\frac{2k_1 I_t}{L\omega_1\rho_1}} \Bigg/ \sqrt{\frac{2k_2 I_t}{L\omega_2\rho_2}} = \sqrt{\frac{k_1\,\omega_2\rho_2}{k_2\,\omega_1\rho_1}} \tag{2}$$

where the subscripts denote the properties of two different soils. Xie and Gough (2013) then propose that Eq. (2) can be indirectly employed in conjunction with Eq. (1) to predict the depth of soil thaw in a two-layered soil using a sequential approach. They first propose that the total thawing index should be used to predict the hypothetical thaw depth if the entire domain were homogeneous with the properties of layer 1 (Eq. 19 of Xie and Gough, 2013):

$$\xi_1 = \sqrt{\frac{2k_1 I_t}{L\omega_1\rho_1}} \tag{3}$$

Xie and Gough (2013) then note that if ξ_1 is less than the thickness of the first layer (Z_1) (Fig. 1a), the algorithm is complete, and $\xi = \xi_1$. If $\xi_1 > Z_1$ (Fig. 1b), a 'residual depth' can be obtained:

$$\Delta\xi_1 = \xi_1 - Z_1 \tag{4}$$

According to Xie and Gough (2013), the thawing depth propagation into the second layer can then be obtained from Eqs. (2) to (4):

$$\xi_2 = \frac{\Delta\xi_1}{P_{12}} \tag{5}$$

Thus, for a two layered thawing soil, the general Xie and Gough (2013) algorithm becomes:

$$\xi = \left\{ \begin{matrix} \sqrt{\frac{2k_1 I_t}{L\omega_1\rho_1}} & \text{if } I_t \leq I_1 \\ Z_1 + \frac{\xi_1 - Z_1}{P_{12}} & \text{if } I_t > I_1 \end{matrix} \right\} \tag{6}$$

where I_1 is the thawing index required to thaw the first layer. This parameter can be obtained by rearranging Eq. (3) and replacing I_t with I_1 and ξ_1 with Z_1.

$$I_1 = \frac{{Z_1}^2 L\omega_1\rho_1}{2k_1} \tag{7}$$

The Xie and Gough (2013) algorithm for a two layered thawing soil can be shown to reduce to Eq. (8) via algebraic manipulation:

$$\xi = \begin{cases} \sqrt{\dfrac{2k_1 I_t}{L\omega_1\rho_1}} & \text{if } I_t \leq I_1 \\ Z_1 + \sqrt{\dfrac{2k_2 I_t}{\omega_2\rho_2 L}} - Z_1\sqrt{\dfrac{k_2\omega_1\rho_1}{k_1\omega_2\rho_2}} & \text{if } I_t > I_1 \end{cases} \tag{8}$$

This algorithm is invalid due to the tacit assumptions of Eq. (5) (Eq. 21 in Xie and Gough, 2013). Most notably this algorithm does not account for the fact that as the thawing front penetrates past the layer interface (Fig. 1b), the upper layer temperature gradient and the layer interface temperature (which drives thawing in the lower layer) become dependent on the lower layer thermal properties. These dependencies arise because both the temperature distribution and the conductive flux must be continuous across the layer interface, even under quasi-steady-state conditions (Lachenbruch, 1959). Thus, $\Delta\xi_1$, which is effectively a measure of the thawing potential for the second layer, cannot be obtained independently of the second layer thermal properties and then directly employed to obtain ξ_2 via Eq. 5. Hence, the assumptions invoked by Eqs. (5) to (8) are not physically tenable even under the limiting conditions of the Stefan approach.

3. The Nixon and McRoberts (1973) equation

A preferable approach for obtaining a modified Stefan equation for two layered soils is to derive the equation from first principles using the governing heat transport equations, boundary conditions, and initial conditions. The unsteady one-dimensional heat diffusion equation for homogeneous soils is (Williams and Smith, 1989):

$$k\frac{\partial^2 T}{\partial z^2} = C\frac{\partial T}{\partial t} \tag{9}$$

where T is temperature (°C), z is depth (m), t is time (s), and C is the volumetric heat capacity of the soil (J m^{-3} $°C^{-1}$). Eq. (9) represents heat diffusion above the thawing front and does not account for the latent heat released or absorbed during the freeze-thaw process. When the rate of temperature change within the subsurface is slow (as in the case of slow downward propagation of the thawing depth), Eq. (9) can be approximated with the steady one-dimensional heat conduction equation:

$$k\frac{d^2 T}{dz^2} = 0 \tag{10}$$

This quasi-steady-state assumption is valid when the Stefan number is low and latent energy exchange dominates sensible energy transfer (Kurylyk *et al.*, 2014a). Eq. (10) implies that since the divergence of the conductive flux is zero, the thermal gradient must be a constant for homogeneous soil. This is also the approach employed in the development of the classic Stefan equation.

If the total thawing index is less than I_1 (see Eq. 7), then the thawing front is within the first layer (Fig. 1a), and it can be calculated via the homogeneous Stefan equation (Eq. 1). This derivation has been frequently presented in geotechnical engineering texts (e.g., Jumikis, 1977).

Equations can be obtained for the interface between the two soil layers. Firstly, the temperature must be continuous across the interface:

$$T_1\big|_{z=Z_1} = T_2\big|_{z=Z_1} \tag{11}$$

where T_1 represents the temperature distribution in the upper layer (°C), T_2 represents the temperature distribution in the lower layer (°C), and Z_1 represents the thickness of the upper layer (m). Also, the conductive flux must be continuous across the layer interface, except when the thawing front is exactly at the layer interface (Lachenbruch, 1959).

$$-k_1 \left.\frac{dT_1}{dz}\right|_{z=Z_1} = -k_2 \left.\frac{dT_2}{dz}\right|_{z=Z_1} \tag{12}$$

Equation (12) indicates that the temperature gradient in the upper layer is dependent on the thermal properties of the lower layer when the thawing front propagates past the layer interface. This complicates the governing equations as has been previously noted in the derivation of solute transport analytical solutions for layered soils, which are governed by analogous physics and mathematics (e.g., Pérez Guerrero *et al*., 2013).

If there is a negligible conductive flux below the thawing front (i.e. thermally uniform conditions close to 0°C), the conductive flux immediately above the thawing front is equal to the rate of latent heat absorbed at the thawing front. In the case when the thawing front penetrates past the layer interface, this energy balance can be written as:

$$-k_2 \frac{dT_2}{dz} = \omega_2 \rho_2 L \frac{d\xi}{dt} \quad . \tag{13}$$

When the thawing front is in the second layer, the heat fluxes in the upper and lower (but still above the thawing front) layers are related to the temperatures at the surface, layer interface, and thawing front:

$$-k_1 \frac{dT_1}{dz} = -k_1 \frac{T_Z - T_s}{Z_1} \tag{14}$$

$$-k_2 \frac{dT_2}{dz} = -k_2 \frac{T_f - T_z}{\xi - Z_1} \tag{15}$$

where T_s is the surface temperature for a given time (°C), T_f is the freezing temperature (0°C), and T_Z is the temperature at the layer interface (°C). Equating (14) and (15) due to the conductive flux continuity condition (Eq. 12), dropping the null T_f term, and rearranging to isolate for T_Z yields:

$$T_Z = \frac{k_1 T_s}{\left(\frac{Z_1 k_2}{\xi - Z_1}\right) + k_1} . \tag{16}$$

Eqs. (15) and (16) can be combined to provide an expression for the conductive flux above the thawing front:

$$-k_2 \left.\frac{dT_2}{dz}\right|_{z=Z_1} = \frac{k_2\, k_1 T_s}{Z_1 k_2 + k_1 \xi - k_1 Z_1} . \tag{17}$$

This conductive flux is equal to the rate of latent heat absorbed at the thawing front in accordance with Eq. (13).

$$\frac{k_2\, k_1 T_s}{Z_1 k_2 + k_1 \xi - k_1 Z_1} = \omega_2 \rho_2\, L \frac{d\xi}{dt} \tag{18}$$

Rearranging to integrate yields:

$$\frac{k_2\, k_1}{\omega_2 \rho_2\, L} \int_{t_1}^{t} T_s\, dt = \int_{Z_1}^{\xi} \left(Z_1 k_2 + k_1 \xi - k_1 Z_1\right) d\xi \tag{19}$$

The lower limits of integration indicate that the integration begins when the depth to the thawing front crosses the layer interface depth (Z_1), which occurs at $t = t_1$.

Integrating Eq. (19) and recalling the fundamental definition of the total thawing index (see Fig.1) yields:

$$\frac{k_2\, k_1}{\omega_2 \rho_2\, L}\left(I_t - I_1\right) = \left(Z_1 k_2 \xi + \frac{k_1 \xi^2}{2} - Z_1 k_1 \xi\right) - \left(Z_1^{\ 2} k_2 - \frac{k_1 Z_1^{\ 2}}{2}\right) \tag{20}$$

Eq. (20) can be rearranged into the format of the quadratic equation with ξ as the variable:

$$\frac{k_1 \xi^2}{2} + \left(k_2 - k_1\right) Z_1 \xi - \left(Z_1^{\ 2} k_2 - \frac{k_1 Z_1^{\ 2}}{2} + \frac{k_2\, k_1}{\omega_2 \rho_2\, L}\left(I_t - I_1\right)\right) = 0 \tag{21}$$

Applying the quadratic equation yields:

$$\xi = \frac{-Z_1\left(k_2 - k_1\right) \pm \sqrt{\left(Z_1 k_2 - Z_1 k_1\right)^2 + \dfrac{2k_2\, k_1^{\ 2}}{\omega_2 \rho_2\, L}\left(I_t - I_1\right) + \left(2k_1 k_2 Z_1^{\ 2} - k_1^{\ 2} Z_1^{\ 2}\right)}}{k_1} \tag{22}$$

I_1 can be obtained from Eq. (7). If $I_t = I_1$ then $\xi = Z_1$, and it is trivial to employ this condition to restrict the solution (Eq. 22) to the positive root. Expanding terms, simplifying, and recalling that the classic Stefan equation is valid when the thawing front is in the first layer yields the final version of the modified Stefan equation for two-layered soils:

$$\xi = \begin{cases} \sqrt{\dfrac{2k_1\, I_t}{L \omega_1 \rho_1}} & \text{if } I_t \le I_1 \\ -Z_1 \dfrac{k_2}{k_1} + Z_1 + \sqrt{\dfrac{Z_1^{\ 2} k_2^{\ 2}}{k_1^{\ 2}} + \dfrac{2k_2\, I_t}{\omega_2 \rho_2\, L} - \dfrac{Z_1^{\ 2} k_2 \omega_1 \rho_1}{k_1 \omega_2 \rho_2}} & \text{if } I_t > I_1 \end{cases} \tag{23}$$

Note that I_t still refers to the total thawing index since $t = 0$ (Fig. 1), not simply the thawing index from the time the thawing front passes the first layer. This methodology can be expanded to accommodate soil with more than two layers, as each additional layer introduces new unknowns (e.g., temperature distribution in *nth* layer) and new boundary conditions (temperature and flux continuity across the layer interface). It will eventually become more practical to use numerical methods if the soil is broken up into many layers. Both Eqs. (8) and (23) expectedly reduce to the Stefan equation for homogeneous soils (Eq. 1) if $\omega_1=\omega_2$, $\rho_1 = \rho_2$ and $k_1 = k_2$. However, these equations can diverge greatly if the thermal conductivities and/or the moisture contents differ between layers.

After deriving Eq. (23), I noticed that this equation was already proposed several decades ago by Nixon and McRoberts (1973). The forms of these equations (i.e., Eq. 23 here and Eq. 19 of Nixon and McRoberts, 1973) can be shown to be identical when adjustments are made for the different nomenclatures employed. Only the governing equations and boundary conditions were presented by Nixon and McRoberts (1973), and thus I thought it valuable to include the derivation presented above to demonstrate the physical basis for this formulation.

Furthermore, Eq. (23) can be shown to be identical to the multi-layered Stefan approach developed by Aldrich and Paynter (1953) (at least in the case of a two-layered thawing soil), although these two approaches were developed using very different techniques. This is the algorithm which is presented in Jumikis (1979, p. 216-219) and Woo (2012, p. 55) and which was criticized by Xie and Gough (2013). For example, this equation in the case of two layered soils is (from Eqs. 9 and 10 of Xie and Gough, 2013):

$$\xi = Z_1 - k_2 R_1 + \sqrt{{k_2}^2 {R_1}^2 + \frac{2k_2 I_2}{L\omega_2\rho_2}} \tag{24}$$

where R_1 is the thermal resistance in layer 1 (i.e., thickness of layer divided by thermal conductivity) and I_2 is the thawing index (°C s) not consumed in the thawing of layer 1 ($I_t - I_1$). Substituting the expressions in for R_1 and I_2 yields:

$$\xi = Z_1 - Z_1 \frac{k_2}{k_1} + \sqrt{\frac{k_2{}^2 Z_1{}^2}{k_1{}^2} + \frac{2k_2\left(I_{th} - I_1\right)}{L\omega_2\rho_2}} \quad (25)$$

which can be shown to be equivalent to Eq. (23) via the definition of I_1 given in Eq. (7). It should be noted, however, that some texts appear to define I_2 as the thawing index required to freeze the *entire* last layer that experiences thaw in a multi-layered soil (i.e., in this case the entire second layer), whereas herein it is physically defined as the thawing index not consumed by the thawing of the preceding layer(s).

4. Assessment of solution via numerical methods

Numerical methods can be employed to demonstrate that the solution form originally presented by Nixon and McRoberts (1973), and derived herein as Eq. (23), is able to reproduce the physics of soil thawing in two-layered soils, at least under the remaining assumptions of the Stefan approach. SUTRA is a finite element model that simulates groundwater flow and coupled heat or solute transport in soils (Voss and Provost, 2010). A beta version of the code allows for soil freezing and thawing (McKenzie *et al.*, 2007) and has been applied to study the hydraulic and thermal regimes of permafrost and seasonally freezing soils (e.g., Briggs *et al*., 2014; Ge *et al*., 2011; Kurylyk *et al*., 2014b; McKenzie and Voss, 2013; Wellman *et al*., 2013). Readers are directed to these papers for a description of the underlying equations and numerical solution techniques employed in this version of SUTRA.

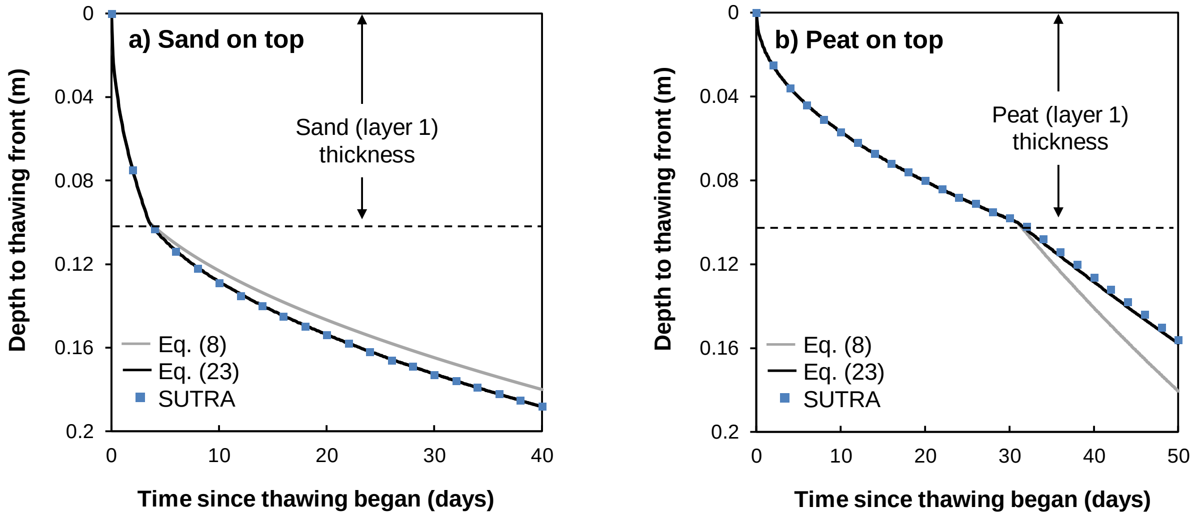

Figure 2: Soil thaw penetration into a two-layered soil for (a) sand overlying peat and (b) peat overlying sand as predicted by the Xie and Gough (2013) algorithm (Eq. 8), Nixon and McRoberts (1973) equation (Eq. 23), and SUTRA simulation. Parameters for the numerical and analytical solutions are given in Table 1.

SUTRA simulations were performed for two simple hypothetical soil thawing scenarios. In the first scenario, a 10 cm thick (Z_1, Fig. 1) layer of saturated sand with a porosity of 0.4 overlies a 10 cm thick layer of saturated peat with a porosity of 0.8. In the second scenario, the peat soil occupies the 10 cm upper layer, and the sand is below. The soil properties for these thawing scenarios are given in Table 1 and are taken from Monteith and Unsworth (2007) for these soil types.

SUTRA parameters are also listed in Table 1. Short time steps (0.0001 days) and small elements (a column of 200 elements with 1 mm height) were used due to the non-linearity of the equations and the steep freezing curve employed (see Kurylyk *et al.*, 2014a). Specified pressure boundary conditions were established so that no groundwater flow occurred, and thus heat advection was negligible. A specified temperature (1 °C) was assigned to the surface of the soil column. In accordance with the Stefan equation, no lower thermal boundary condition was assigned. The specific heats for the peat and sand were set to a low value (0.1 J kg^{-1} °C^{-1}) to mimic the quasi-steady conditions of the Stefan approach.

Table 1: Parameterization of analytical solutions and SUTRA

Symbol	Definition	Value	Units
k_1	Sand conductivity	0.5	W m^{-1} °C^{-1}
k_2	Peat conductivity	2.2	W m^{-1} °C^{-1}
L	Latent heat of fusion	3.34E5	J kg^{-1}
Z_1	Thickness of layer 1	0.10	m
T_s	Surface temp.[1]	1	°C
$\omega_1\rho_1$	See note[2]	800	kg m^{-3}
$\omega_2\rho_2$	See note[2]	400	kg m^{-3}
Δt	SUTRA time step size	0.0001	days
Δz	SUTRA element height	0.001	m
T_m	Thawing curve min[3]	-0.005	°C

[1]The surface temperature was constant, thus the thawing index is equal to 1°C × time.
[2] For saturated soils, the product of the moisture content by weight and the dry bulk density can be shown to be equal to the porosity times the density of bulk water.
[3] The analytical solutions consider thawing to occur at a single temperature, but in SUTRA freezing and thawing occur over a temperature range. T_m is the temperature at which the soil is fully frozen. The soil freezing curve was linear (Kurylyk *et al*., 2014a). Initial conditions were set at T_m (-0.005 °C) to ensure that the soil was fully frozen.

Figure 2 demonstrates that the SUTRA simulations concur with Eq. (23) proposed by Nixon and McRoberts (1973) rather than Eq. (8) developed by Xie and Gough (2013). For both thawing scenarios, the analytical and numerical solutions overlap until the thawing front has penetrated past the depth of the first layer, but the curves diverge after this point. In the scenario with sand on top (Fig. 2a), the difference between Eq. (23) and Eq. (8) after 40 days is 8 mm (4.5%), and the difference between Eq. (23) and the SUTRA results is less than the element size (1 mm). In the scenario with peat on top, the difference between Eq. (23) and Eq. (8) after 50 days is -23 mm (-14%), whereas the difference between Eq. (23) and SUTRA is only 1.8 mm (1%). The minor discrepancies between the SUTRA results and Eq. (23) in Fig. 2 can be attributed to spatiotemporal discretization errors and the finite freezing temperature range employed.

In summary, Eqs. (23) or (24) should be utilized for parsimonious analyses of layered soils rather than the Xie and Gough (2013) algorithm or the homogenous Stefan equation (1), as the former is not mathematically correct and the latter can produce significant errors in multi-layered soils. This is particularly the case in many permafrost regions where a layer of insulating peat overlies a more thermally conductive soil or in locations where a thin pavement layer with distinct thermal properties overlies a homogeneous soil (e.g., Jumikis, 1977, p. 217). Furthermore, Eq. (23) may prove to be useful in calculating the influence of segregated ice on the thawing rate of otherwise relatively homogeneous soil. Modified Stefan algorithms for layered soils can be incorporated into cold regions hydrology and land surface models to estimate the frost depth or active layer depth in heterogeneous soils (Carey and Woo, 2005; Fox, 1992; Woo *et al.*, 2004).

5. Conclusions

It is not my intent to discount the interesting paper by Xie and Gough (2013). Indeed there are many valuable aspects of that paper including their soil freeze-thaw data from sites in China and the discussion related to the importance of including more flexible soil freeze-thaw algorithms in cold regions hydrology and land surface models. The intent of this discussion was to rather identify and explain the implicit errors in their algorithm and then to direct land surface and cold regions hydrology modelers back to the Nixon and McRoberts (1973) equation (herein Eq. 23), which is more rigorously derived and has been verified with numerical methods.

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