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Short Communication
A Simple Thaw-Freeze Algorithm for a Multi-Layered Soil using the Stefan Equation

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ABSTRACT

The Stefan equation is one of the simplest approximate analytical solutions for the thaw-freeze problem. It provides a useful method for predicting the depth of thawing/freezing in soils when little site-specific information is available. The limited number of parameters in the Stefan equation makes possible its application in a multi-layered system. We demonstrate that a widely used algorithm (JL-algorithm), which has been frequently used in permafrost regions, was derived by an incorrect mathematical method. It will inevitably result in systematic errors in the simulation if this algorithm is used in a multi-layered soil.
We present another simple thaw-freeze algorithm (XG-algorithm) for multi-layered soils. The new algorithm can be used to determine the freeze/thaw front in multi-layered soils no matter how thick each layer is and how many layers the soil profile contains. Simulation results of the JL-algorithm and the XG-algorithm are compared using hypothetical soil profiles, and the XG-algorithm is also used to simulate the thaw depth at three permafrost monitoring sites on the Qinghai-Tibet Plateau and one on the Loess Plateau, China. These applications show that the XG-algorithm could be readily used to analyse the factors that affect active-layer thickness. It can also be coupled with hydrological or land surface models to simulate the freeze-thaw cycles in permafrost regions and for related engineering applications.

KEY WORDS: Stefan equation; algorithm; thaw-freeze depth; multi-layered soil; permafrost

INTRODUCTION

The Stefan equation was originally derived to predict the growth in thickness of a single ice sheet over calm polar water (Stefan, 1891) and has been applied to the freezing of water in a porous material by Berggren (1943) (quoted by Holden *et al*., 1981). The equation provides a useful method for predicting the depth of freezing and thawing in soils where little site-specific information is available (Nelson *et al*., 1997; Woo *et al*., 2004). During the last several decades, the Stefan equation has been widely used for spatial active-layer characterisation by estimating soil properties empirically, using air temperature records and active-layer thickness (ALT) obtained from representative locations (Riseborough *et al*., 2008). However, in most of those studies, the soil profile is modelled either as a homogeneous medium or the properties of different soil layers are averaged over the full thickness of the active layer (Romanovsky and Osterkamp, 1997; Nelson *et al*., 1997; Gough and Leung, 2002; Shiklomanov and Nelson, 2003; Zhang *et al*., 2005; Pang *et al*., 2006; Yang and Chen, 2011). These treatments have inevitably caused errors in the simulation results. For example, systematic errors of up to 71 per cent had been found when the Stefan equation was used to predict ALTs in two-layered or three-layered active layers on the Alaskan Arctic Coastal Plain (Romanovsky and Osterkamp, 1997).

Some efforts to use the Stefan equation in a multi-layered system have been made, especially for engineering applications (Jumikis, 1977; Lunardini, 1981), although the original Stefan equation was derived for a homogeneous medium. The equation was used in a multi-layered system to simulate the frost penetration below highway and airfield pavements as early as 1956 by Aldrich (1956) (quoted by Holden *et al*., 1981). The numerical algorithm was

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introduced in detail by Jumikis (1977) and Lunardini (1981) and thereafter has been used frequently. In this algorithm (abbreviated as JL-algorithm), which is also referred to as the St Paul equations in some papers (Kersten, 1959) (quoted by Lunardini, 1981; Fox, 1992), the freezing (or thawing) depth is calculated by evaluating the partial freezing (or thawing) index of the total surface freezing (or thawing) index that is necessary to freeze (or thaw) each soil layer. Nelson and Outcalt (1987) used this algorithm as a computational method to analyse the distribution of permafrost. Fox (1992) incorporated this algorithm into a water balance model. Woo *et al*. (2004) modified the algorithm by inverting the equations and driving the algorithm in two directions using temperatures at both the surface and at a specified depth in the soil column. The improved algorithm has also been incorporated into the Terrestrial Ecosystem Model to simulate the thermal and hydrological dynamics within soil profiles that contain several layers (Yi *et al*., 2009; Yi *et al*., 2007). However, by examining the mathematical formulation of the JL-algorithm, we found that this algorithm was derived by an incorrect mathematical method. It will inevitably result in systematic errors in the simulation results if this algorithm is used in a multi-layered soil in which each layer has different physical parameters.

In this paper, we present another simple thaw-freeze algorithm, hereafter referred to as the XG-algorithm, for multi-layered soils. The XG-algorithm can be used to determine the freezing (or thawing) depth no matter how thick each layer is and how many layers the soil profile contains. Simulation results of both the JL- and XG-algorithms are discussed using three hypothetical soil profiles. The XG-algorithm is also used to simulate the thaw depth at three permafrost monitoring sites on the Qinghai-Tibet Plateau and one on the Loess Plateau (China). Practicality and accuracy of this algorithm are tested and it is shown that the XG-algorithm can be reliably used to analyse these factors that affect the ALT.

THE JL-ALGORITHM

The Stefan equation provides an approximate solution to heat conduction under the assumption that sensible heat effects are negligible. The common form of the Stefan equation (Jumikis, 1977) is:

$$\xi = \left(\frac{2k\cdot F}{Q_L}\right)^{0.5} = \left(\frac{2k\cdot F}{L\cdot\omega\cdot\rho}\right)^{0.5} \tag{1}$$

where ξ is the freeze/thaw depth, k is the thermal conductivity ($W/(m\cdot K)$) of the soil, F is the surface freeze/thaw index, in C degree-days, Q_L is the volumetric latent heat of soil, in J/m^3, and $Q_L = L\cdot\omega\cdot\rho$ where L is the latent heat of fusion of ice (3.35×10^5 J/kg), ω is the water content, as a decimal fraction of the dry soil weight, and ρ is the bulk density of the soil (kg/m^3).

The following introduction of the JL-algorithm was in accordance with Jumikis (1977, pp 218–219).

By squaring the Stefan equation, we derive:

$$\xi^2 = \frac{2k\cdot F}{Q_L} \tag{2}$$

Now, differentiating the squared Stefan equation:

$$2\xi\cdot\Delta\xi = \frac{2k\cdot\Delta F}{Q_L} \tag{3}$$

ΔF is expressed from Equation 3 as:

$$\Delta F = (Q_L\cdot\Delta\xi)\cdot\left(\frac{\xi}{k}\right) \tag{4}$$

where ξ is the total frost/thaw penetration depth into a multi-layered soil system, $\Delta\xi$ is the frost/thaw penetration depth increment, known also as the partial frost/thaw penetration, and ΔF is the partial freezing/thawing index, in degree-days, to bring about a corresponding partial frost/thaw penetration in any one layer.

Setting $\Delta F = N_i$ which are the degree-days required at the surface to move the 0 °C isotherm through a soil layer $\Delta\xi = z_i$ unit thick, and substituting $\Delta\xi/k_\xi = z_i/k_i = R_i$ which is the thermal resistance of soil of thickness z_i, Equation 4 is rewritten as:

$$N_i = (Q_{Li}\cdot z_i)\cdot\left(\frac{z_i}{k_i}\right) = (Q_{Li}\cdot z_i)\cdot\left(\frac{R_i}{2}\right) \tag{5}$$

Observe that in these calculations, R_i is taken at the midpoint of the layer, hence $R_i/2$ in Equation 5. To obtain the partial surface index, N_i, for each layer required to penetrate the 0 °C isotherm through a soil layer z_i unit thick, we proceed by Equation 5 as follows:

For the first layer, $z_i = z_1$ units thick:

$$N_1 = (Q_{L1}\cdot z_1)\cdot\left(\frac{R_1}{2}\right) \tag{6}$$

For the second layer, $z_i = z_2$ units thick:

$$N_2 = (Q_{L2}\cdot z_2)\cdot\left(R_1 + \frac{R_2}{2}\right) \tag{7}$$

Analogous to this law, for the n^{th} layer, $z_i = z_n$ units thick:

$$N_n = (Q_{Ln}\cdot z_n)\cdot\left(\sum_{i=1}^{n-1} R_i + \frac{R_n}{2}\right) \tag{8}$$

where $\sum_{i=1}^{n-1} R_i$ is the thermal resistance of all of the layers above the n^{th} layer, and R_n is the thermal resistance of the n^{th} layer. The total degree-days used, F, is equal to $N_1 + N_2 + \ldots N_n$.

From Equation 8, the freezing/thawing depth ξ_{fn+1} into layer $n+1$ of the soil is calculated from the quadratic equation as:

$$\xi_{n+1} = -k_{n+1}\sum_{i=1}^{n} R_i + \left\{k_{n+1}^2\left[\sum_{i=1}^{n} R_i\right]^2 + \left[\frac{2k_{n+1}N_{n+1}}{Q_{Ln+1}}\right]\right\}^{0.5} \tag{9}$$

The total freezing depth ξ is equal to:

$$\xi = \sum_{i=1}^{i=n} z_i + \xi_{n+1} \tag{10}$$

The above mathematical derivations are based on the differential form of the squared Stefan equation. Theoretically, only the continuity equation can be differentiated and has a differential form. In Equation 2, if ξ and F are the variables, k and Q_L should be constants, or k/Q_L should be constant. However, this is not true at the interface of two soil layers with different physical parameters (except for special conditions, i.e. $k_i/Q_{Li} = \text{constant}$). In a multi-layered soil in which every layer has different physical parameters (Figure 1), the temperature gradient varies in different soil layers. There is no standard continuity equation for the relationship of ξ and F when the freezing/thawing front moves across the interface of two layers with different physical parameters. As a result, we cannot derive the JL-algorithm in a multi-layered soil based on the differential form of the squared Stefan equation.

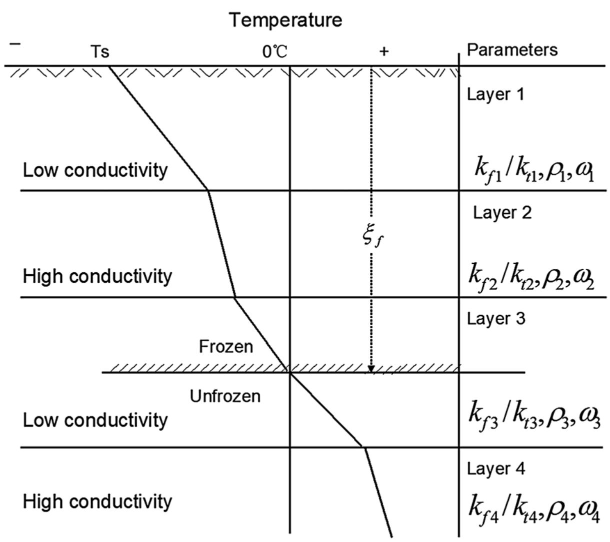

Figure 1 Influence of physical parameters on the geothermal gradient. T_s is the surface temperature while other symbols in the figure have same meaning as that in the text. Suffix *f* and *t* are corresponding to the freeze and thaw conditions, separately, and the suffix numbers are corresponding to the layer number. (from Williams and Smith, 1989).

However, the JL-algorithm can be obtained by a relatively simple mathematical method in a homogeneous soil. Consider a homogeneous soil (thickness z) which is divided into n layers, for example, layer 1 (thickness z_1), layer 2 (thickness z_2), layer 3 (thickness z_3) and so on. Definitions of N_i and R_i are the same as those given by Jumikis (1977). If the freezing/thawing depth, ξ, is equal to z_1, the total degree-days can be calculated as:

$$F_{z_1} = \frac{Q_L}{2k}\cdot(z_1)^2 = Q_L z_1\left(\frac{R_1}{2}\right) = N_1 \tag{11}$$

If $\xi = z_1 + z_2$, the following relationship exists:

$$\begin{aligned} F_{z_1+z_2} &= \frac{Q_L}{2k}\cdot(z_1+z_2)^2 = \frac{Q_L}{2k}\left(z_1^2 + 2z_1\cdot z_2 + z_2^2\right) \\ &= Q_L\cdot z_1\cdot\left(\frac{R_1}{2}\right) + Q_L\cdot z_2\cdot(R_1) + Q_L\cdot z_2\cdot\left(\frac{R_1}{2}\right) \\ &= Q_L\cdot z_1\cdot\left(\frac{R_1}{2}\right) + Q_L\cdot z_2\cdot\left(R_1 + \frac{R_1}{2}\right) \\ &= N_1 + N_2 \end{aligned} \tag{12}$$

For $\xi = z_1 + z_2 + z_3 + \cdots + z_n$, we obtain:

$$\begin{aligned} F_{z_1+\cdots+z_n} &= \frac{Q_L}{2k}\cdot(z_1 + z_2 + \cdots + z_n)^2 \\ &= \frac{Q_L}{2k}\cdot\Big(z_1^2 + z_2^2 + \cdots z_n^2 + 2z_1\cdot z_2 + 2z_1\cdot z_3 \\ &\quad + \cdots 2z_1\cdot z_n + \cdots 2z_{n-1}\cdot z_n\Big) \\ &= Q_L z_1\cdot\left(\frac{R_1}{2}\right) + Q_L z_2\cdot\left(R_1 + \frac{R_2}{2}\right) \\ &\quad + Q_L z_3\cdot\left(R_1 + R_2 + \frac{R_3}{2}\right) + \cdots \\ &\quad + (Q_L\cdot z_n)\cdot\left(\sum_{i=1}^{n-1} R_i + \frac{R_n}{2}\right) \\ &= N_1 + N_2 + N_3 + \cdots + N_n \end{aligned} \tag{13}$$

and

$$N_n = Q_L\cdot z_n\cdot\left(\sum_{i=1}^{n-1} R_i + \frac{R_n}{2}\right) \tag{14}$$

Thus, from the standard Stefan equation we derived the same equation (Equation 14) as that in Equation 8. In our mathematical derivation, both k and Q_L are constants in different soil layers. But since k and Q_L are seldom constants in natural multi-layered soils, the resulting depth will differ. Unless k and Q_L are constants in different soil layers, we cannot generate the same equation. This derivation illustrates that the JL-algorithm was derived for a multi-layered soil in which every layer has the same physical parameters (i.e. in a homogeneous soil). In conclusion, the JL-algorithm cannot be used on a multi-layered soil in which each layer has different physical parameters.

THE XG-ALGORITHM FOR A MULTI-LAYERED SOIL

The XG-algorithm provides a new, simple algorithm that applies the Stefan equation to calculate the freezing (or thawing) depth in a multi-layered soil in which every layer has different physical parameters. It avoids the pitfalls of averaging the soil parameters in a multi-layered soil, and is independent of layer thickness and number. In a two-layered or three-layered soil, it only needs a few additional steps to calculate the thawing/freezing depth by the Stefan equation. This algorithm can be used in ALT simulations in permafrost regions.

For a given surface freeze/thaw index, the thaw/freeze depth of two soil types (types A and B, indicated below by a suffix a or b) in the same locality can be calculated by the Stefan equation:

$$\xi_a = \left(\frac{2k_a \cdot F}{Q_{La}}\right)^{0.5} = \left(\frac{2k_a \cdot F}{L \cdot \omega_a \cdot \rho_a}\right)^{0.5} \tag{15}$$

$$\xi_b = \left(\frac{2k_b \cdot F}{Q_{Lb}}\right)^{0.5} = \left(\frac{2k_b \cdot F}{L \cdot \omega_b \cdot \rho_b}\right)^{0.5} \tag{16}$$

The following relationship exists:

$$P_{ab} = \frac{\xi_a}{\xi_b} = \left(\frac{2k_a \cdot F/(L \cdot \rho_a \cdot \omega_a)}{2k_b \cdot F/(L \cdot \rho_b \cdot \omega_b)}\right)^{0.5} = \left(\frac{k_a \cdot \rho_b \cdot \omega_b}{k_b \cdot \rho_a \cdot \omega_a}\right)^{0.5} \tag{17}$$

The ratio P_{ab} only depends on the physical parameters of the two soil types, independent of the freeze/thaw index value. For a given freeze/thaw index, if we know the freezing/thawing depth of type A soil, the freezing/thawing depth of type B can be deduced:

$$\xi_b = \frac{\xi_a}{P_{ab}} \tag{18}$$

Analogous to this, the total freezing/thawing depth can be calculated in an actual soil profile that is formed by more than two layers, for example, layer 1 (thickness z_1), layer 2 (thickness z_2), layer 3 (thickness z_3) and so on. Firstly, we assume that the entire soil column is homogeneous with the same soil physical properties as that of layer 1. For a given value of F, the freezing/thawing depth in this virtual soil profile can be calculated by the Stefan equation:

$$\xi_1 = \left(\frac{2k_1 \cdot F}{\rho_1 \cdot \omega_1 \cdot L}\right)^{0.5} \tag{19}$$

If $\xi_1 \le z_1$, the freezing/thawing front is in layer 1 and the calculation is complete. The real freezing/thawing depth is equal to ξ_1. If $\xi_1 > z_1$, which means the freeze/thaw index is more than that needed to freeze/thaw the actual first layer, the residual depth can be calculated as follows:

$$\Delta\xi_1 = \xi_1 - z_1 \tag{20}$$

Secondly, we assumed that there is another virtual soil profile whose entire profile is formed by the layer 2 soil below layer 1. By Equation 18, it is straightforward to determine the depth of frozen/thawed material in the second virtual soil profile by the freeze/thaw index that was used to freeze/thaw the first soil type with thickness $\Delta\xi_1$:

$$\xi_2 = \frac{\Delta\xi_1}{P_{12}} \tag{21}$$

P_{12} can be determined by the same method as for P_{ab}. If $\xi_2 \le z_2$, the freezing/thawing front is in layer 2 and the calculation is complete. The total freezing/thawing depth equals to $z_1 + \xi_2$. If $\xi_2 > z_2$, the freeze/thaw index is more than that required to freeze/thaw the sum of layer 1 and layer 2, and thus the freezing/thawing front is in the third virtual layer and can be determined by the same method:

$$\Delta\xi_2 = \xi_2 - z_2 \tag{22}$$

$$\xi_3 = \frac{\Delta\xi_2}{R_{23}} \tag{23}$$

Through repeating these steps, the freezing/thawing depth can be determined. If $\xi_{n+1} \le z_{n+1}$, the sum of the freezing/thawing thickness is:

$$\xi = \sum_{i=1}^{i=n} (z_i) + \xi_{n+1} \tag{24}$$

In the special case where every soil layer has identical physical parameters, the ratio, P_{12}, $P_{23,}$ is equal to 1, and this algorithm produces the same results as the original Stefan equation used for a homogeneous soil.

COMPARISON OF XG- AND JL-ALGORITHMS ON HYPOTHETICAL SOIL PROFILES

It is difficult to verify the XG-algorithm in a multi-layered soil because the original Stefan equation on which it is based cannot be used directly in a multi-layered soil. Here, we compare the simulation results of both the XG-algorithm and the JL-algorithm using three hypothetical soil profiles and then discuss how these results reflect changes in the physical properties of a multi-layered soil.

The physical parameters of three soil profiles, each with two layers, are given in Table 1. Profile 1 is a homogeneous silty soil whose properties are constant with depth. Profile 2 comprises an upper layer of peat (which always has high water content and low thermal conductivity) above a lower layer of silt; this structure is a common feature of the active layer in arctic tundra regions. Profile 3 comprises a silt layer above a peat layer. In order to facilitate their comparison, the same daily surface temperature data series are used in the three cases and are given by a cosine function as follows (x is the date, from 1 to 365):

$$T_x = -15 \cdot \cos\left(\frac{2\pi \cdot x}{365}\right) - 3. \quad (25)$$

The total thawing index is 1230 degree-days, and the total thawing period is 160 days. Here, we analyse the thawing process alone. The simulation time step is 1 day. Only a one-directional freeze-thaw regime was considered in these simulations in order to facilitate discussion.

Figure 2 shows the simulation results of both the XG-algorithm and JL-algorithm. In case 1 (Figure 2a), both algorithms have the same results, as expected, which indicates that both algorithms can be used in a multi-layered soil in which each layer has the same physical parameters. In cases 2 and 3 (Figure 2b, c), the results in the first layer are the same but differ in the second. In case 2, the thawing depth calculated by the XG-algorithm is deeper than that calculated by the JL-algorithm, while the opposite is true in case 3. The difference in the maximum thawing depth reached is 0.09 m and 0.08 m, respectively. The curve of the JL-algorithm is smoother than the XG-algorithm. There are no abrupt changes in gradient in the former when the thawing front moves through the interface between the two different layers, which are not consistent with the actual thawing process. Generally, the temperature gradient abruptly changes at the interface of two layers (Figure 1) and thawing should have different characteristics in different soils. The simulation results of the XG-algorithm are more reflective of the physical properties of multi-layered soils. The thawing rate accelerated when the thawing front moved from the low-conductivity soil (peat layer) to the high-conductivity soil (silt layer, case 2), whereas it slowed down in the opposite situation (case 3). From these simulations, we conclude that the JL-algorithm should not be used in a multi-layered soil.

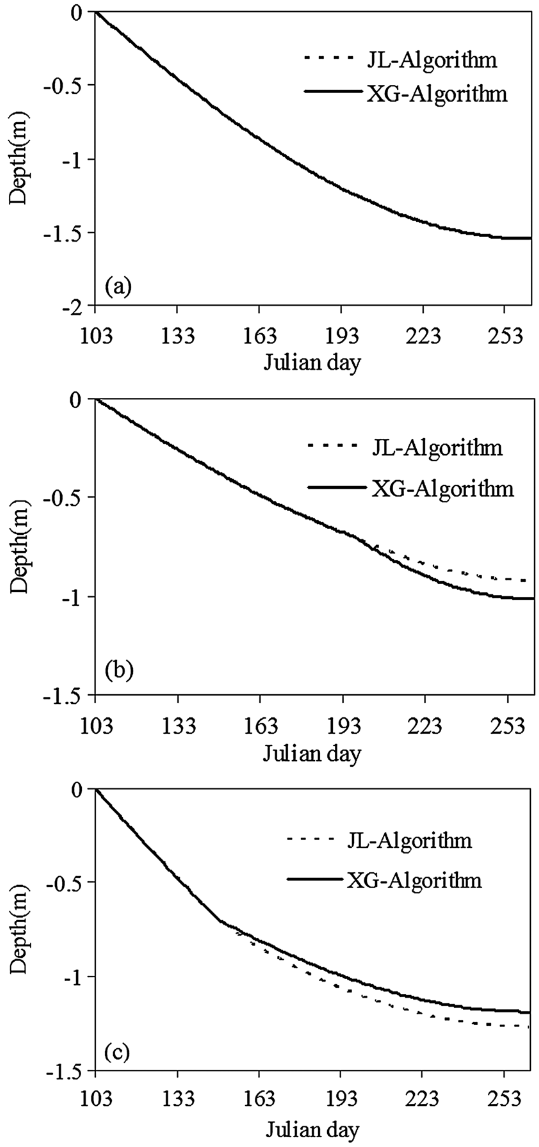

Figure 2 Simulation results of the XG-algorithm and JL-algorithm.

Table 1 Physical parameters of three two-layered soil profiles.

Profile No.	Soil type	Depth of soil layer (m)	Bulk density (kg · m^{-3})	Gravimetric water content	Unfrozen thermal conductivity (W/(m · K))
Case 1	Silt	0.0–0.7	1300	0.30	1.57
	Silt	0.7–2.0	1300	0.30	1.57
Case 2	Peat	0.0–0.7	680	0.70	0.57
	Silt	0.7–2.0	1300	0.30	1.57
Case 3	Silt	0.0–0.7	1300	0.30	1.57
	Peat	0.7–2.0	680	0.70	0.57

Freeze-thaw processes are complex. In permafrost regions, the ALT, for example, is controlled by many factors, including air temperature, vegetation, snow cover, soil moisture, the physical and thermal properties of the surface cover and substrate, organic layer thickness and surface morphology, although the most important factor is usually summer air temperature (Zhang *et al*., 2005). The Stefan equation provides a simple relationship between the freezing/thawing index and the freezing/thawing depth based on the assumption that the latent heat of phase change in the soil layer is much larger than the sensible heat (Jumikis, 1977). It ignores convective heat flow from precipitation, snow melt, and surface water, which, though often negligible, can be an important factor in soil freezing/thawing (Bonan, 1989). Hence, simulation results using the Stefan equation are an approximation compared to the actual observed freezing/thawing depth. Improvements to this formulation must be considered carefully and be based on sound physical and mathematical foundations. The JL-algorithm was derived for limited conditions (i.e. homogeneous soils). We cannot apply it to a multi-layered soil in which every layer has different physical parameters, although the simulation results may sometimes fortuitously be close to the actual observed values. The XG-algorithm has a sound theoretical basis and should be useful to determine the freezing/thawing front in a multi-layered soil. To demonstrate this, we now present a field validation of the XG-algorithm.

FIELD VALIDATION

The practicality and accuracy of using the XG-algorithm to simulate the ALT was investigated at three monitoring sites on the Qinghai-Tibet Plateau and at one site on the Mahan Mountain (China), the only region where permafrost persists in the Chinese Loess Plateau (Xie *et al*., 2010). At the four sites, air temperature, surface temperature (except site CH6), volumetric water content and soil temperature at several depths were continuously observed by automated instruments (Zhao *et al*., 2010; Xie *et al*., 2010, 2012). Gravimetric water content, soil density and most of the thermal conductivity were determined in the laboratory. Some of the thermal conductivities were referenced to the empirical values provided in Xu *et al*. (2001). Detailed site descriptions are given in Zhao *et al*. (2010) and Xie *et al*. (2010, 2012). Table 2 summarises the characteristics of these test sites, and Table 3 lists

Table 2 Regional characteristics of the four monitoring sites.

Sites	Location	Place name	MAAT (°C)	PT (°C)	Surface condition
MHS	35°26.4′N 103°34.8′E	Mahan Mountain	−1.74	−0.20	Silt clay, alpine meadow
CH4	31°49.1′N 91°44.2′E	Liandaohe	−2.0	−0.75	Silt and sandy, alpine meadow
CH6	35°37.3′N 94°03.7′E	Kunlun Pass	−5.82	−2.24	Sandy clay, alpine meadow
QT9	35°43.1′N 94°07.5′E	Xidatan	−2.20	−0.62	Sandy clay, alpine grasslands

MAAT = Mean annual air temperature; PT = permafrost temperature, which is measured at the depth of zero annual amplitude of seasonal temperature variation.

Table 3 Physical parameters used for each site.

Sites	Soil type	Depth of soil layer (m)	Bulk density ($kg \cdot m^{-3}$)	Water content (%)		Thermal conductivity (W/(m · K))	
				Volumetric	Gravimetric	Unfrozen	Frozen
MHS	Peat	0.0–0.70	540	63.5	110.6	0.79*	1.38*
	Silt	0.70–1.05	1280	45.5	35.8	1. 55	1.87
	Silt	1.05–2.00	1300	63.5	48.5	1.67	1.95
CH4	Peat	0.0–0.60	670	46.7	78.4	0.73*	1.54*
	Silt	0.60–1.20	1210	39.5	35.7	1.48	1.78
	Silt	1.20–2.00	1250	40.3	33.5	1.69	1.97
CH6	Silt	0.0–0.25	1120	21.5	24.8	1.47	1.67
	Sandy	0.25–2.0	1320	24.5	18.8	1.85*	1.97*
CH9	Silt	0.0–0.20	1170	29.0	25.5	1. 41	1.76
	Silt	0.20–0.90	1205	28.5	23.0	1.73	1.83
	Sandy	0.90–1.20	1420	24.5	17.5	1.87*	1.97*
	Gravel	1.20–2.00	1670	24.0	15.5	1.98*	2.09*

*Referenced to the empirical values provided in Xu *et al*. (2001).

their physical parameters. The water content used in the models was reduced by a default value of 5 per cent since some water was not involved in the freeze-thaw process.

Both one-directional (1-D: freezing from the surface downwards) and two-directional (2-D: freezing both downwards from the ground surface and upwards from the permafrost table) freeze-thaw regimes were simulated. The models were run at a time step of 1 day (24 h) and the simulation period was the whole year of 2010. The surface freezing and thawing indices were used in the simulations at sites MHS, CH4 and QT9. At CH6, the freezing and thawing indices were calculated by the soil temperature at 1-cm depth.

Figure 3 shows variations in daily mean temperatures, the simulated freezing/thawing fronts and 0 °C isotherms estimated from observed ground temperatures. The simulated thaw depths were generally similar to field observations, whereas the simulated freezing depths showed some differences, particularly for the 1-D XG-algorithm. At sites MHS, CH6 and QT9, the simulated thawing times were longer than those observed, while the opposite was true at CH4. At MHS, CH6 and QT9, the bottom of the active layer began to freeze as soon as the surface temperature dropped below 0 °C and the whole active layer froze relatively quickly, while the simulated freezing depth gradually increased over time with the accumulation of the freezing index, which resulted in a long simulated thawing state. At CH4, the observed span of the thaw period was similar to that observed because the latent heat released from the freezing of water within the active layer prolonged freezing. The XG-algorithm does not account for these freeze-thaw effects. The average percentage difference between the observed and calculated values for the 1-D XG-algorithm was 9.25 per cent and the range of values was -1.6 to 17.01 per cent, while for the 2-D XG-algorithm these values were 7.12, 4.83 and 10.20 per cent, respectively. The simulation results were substantially better than those obtained by Pang *et al.* (2006) and Yang and Chen (2011), which differed by about 50 per cent between the observations and simulations. The systematic errors in this study were large at CH6 and QT9, where the active layer has a low soil water content, consistent with the understanding that application of the Stefan equation to dry soil will cause larger errors (Jumikis, 1977). All simulated annual thaw depths of the 2-D XG-algorithm were smaller than those of the 1-D XG-algorithm, especially at CH6, where the

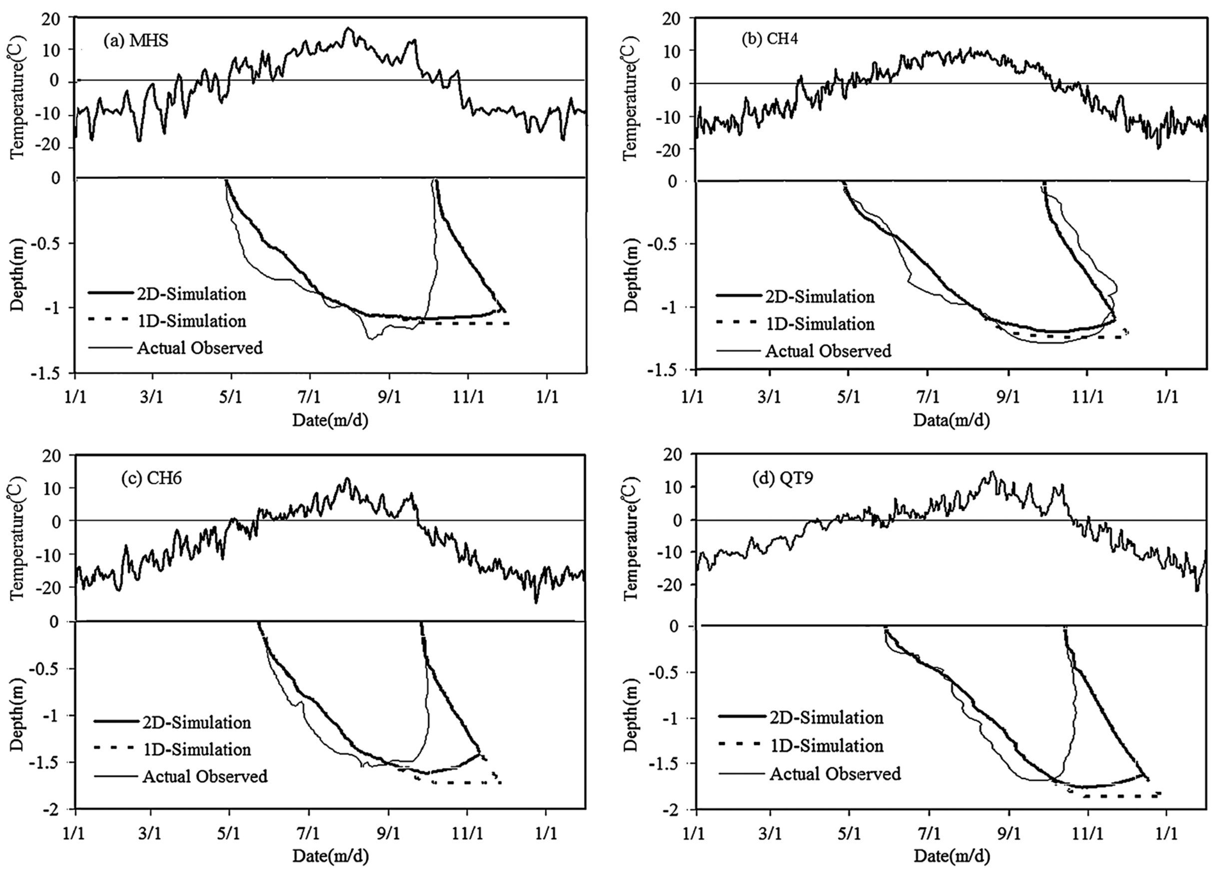

Figure 3 Variations in daily mean surface temperatures (upper), simulated freezing/thawing fronts and 0 °C isotherms (lower) at four monitoring sites in 2010.

Table 4 Simulated depth and systematic errors for 1-D and 2-D XG-algorithms.

Sites	Observed	Simulated depth (m)		Systematic errors (%)	
		1-D	2-D	1-D	2-D
MHS	1.17	1.12	1.07	-4.27	-8.54
CH4	1.25	1.23	1.19	-1.62	-4.83
CH6	1.47	1.72	1.62	17.01	10.20
QT9	1.63	1.86	1.71	14.11	4.91

permafrost temperature is lower than -2.0 °C. The thawing depth simulated by the 2-D XG-algorithm was small because an additional set of equations to drive soil freeze from the bottom was applied. Simulated depths and systematic errors for the 1-D and 2-D XG-algorithms are given in Table 4.

The XG-algorithm accurately simulates the significant impact of air temperature, water content and soil properties on the ALT. For example, the significant thermal impacts of a peat layer are captured by the small simulated ALTs at both sites MHS and CH4, where permafrost has developed in low-lying wetland whose top soil contains organic material such as plant roots and humus. This thick peat layer led to a thin active layer due to low thermal conductivity in summer and larger thermal conductivity in winter. By comparing the simulated and observed ALTs under real conditions and two scenarios (only the 1-D regime was considered in these simulations), the significant impacts of a peat layer can be demonstrated. The first scenario was that the peat layers were reduced to half at MHS and CH4 (i.e. peat layer was 0.35 m at MHS and 0.30 m at CH4), and the reduced part was replaced by soil with the same thermal conductivity and volumetric heat capacity as the second layer. The second scenario was that there was no peat layer at both sites. Simulation results indicated that for the first scenario, the ALT increased by 0.16 m at MHS and 0.12 m at CH4, while for second scenario these values were 0.31 m and 0.25 m, respectively. These simulation results successfully proved that the thick peat layers at MHS and CH4 have the ability to buffer permafrost from thaw, in agreement with the conclusions of Shur and Jorgenson (2007) and Yi *et al.* (2007). The XG-algorithm provides a better method to analyse the impact of soil properties, as well as any other parameters, in different horizons. The successful application of this algorithm showed that the XG-algorithm could be more flexibly used in the permafrost region than the original Stefan equation. It can also be coupled with hydrological and land surface models to simulate freeze-thaw cycles in permafrost regions and for related engineering applications.

CONCLUSIONS

The Stefan equation is one of the simplest approximate analytical solutions for the thaw-freeze problem. The small number of parameters in the equation makes possible its application in a multi-layered system. This work demonstrated that the existing JL-algorithm used by many researchers was derived by an incorrect mathematical method. It will inevitably cause systematic errors in the simulation results when it is used in a multi-layered soil in which each layer has different physical parameters. The XG-algorithm presented here has a sound theoretical basis and is successfully used to determine the freezing/thawing front in multilayered soils. It is straightforward to determine the freezing/thawing front in multi-layered soils no matter how thick each layer is and how many layers the soil profile contains. This successful application indicates that the XG-algorithm could be easily used to analyse those factors that affect ALT. It can also be coupled with hydrological or land surface models to simulate the freeze-thaw cycles in permafrost regions and for related engineering applications.

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