PAPER • OPEN ACCESS

Comparison of analytical solution of the semi-infinite problem of soil freezing with numerical solutions in various simulation software

To cite this article: Andrey Alekseev *et al* 2018 *IOP Conf. Ser.: Mater. Sci. Eng.* **365** 042059

Comparison of analytical solution of the semi-infinite problem of soil freezing with numerical solutions in various simulation software

Andrey Alekseev[1,2], Gleb Gribovskii[3] and Svetlana Vinogradova[2]

[1]Moscow State University of Civil Engineering, Yaroslavskoye shosse, 26, Moscow, 129337, Russia
[2]Research institute of bases and underground structures NIIOSP named after N M Gersevanov, JSC Research Center of Construction, 2nd Institutskaya st., 6, Moscow, 109428, Russia
[3]Department of Theoretical and Applied Mechanics, BSU, Nezavisimosti avenue, 4, Minsk, 220030, Belarus

E-mail: [2] lana_vinogradovaa@list.ru

Abstract. The objective of this research is to determine the most suitable software packages for simulation of thermal effect of various constructions on seasonally frozen or permafrost ground. The abrupt change in soil physical properties at freeze/thaw boundaries is a considerable challenge because it introduces a strong nonlinearity into the heat transfer model. Mathematically speaking, there appears a Stefan condition at the moving boundary of the phase transition. A problem of soil column freezing is considered. The simulation results, obtained by different software, are compared with the analytical solution of the corresponding semi-infinite Stefan problem. The frost penetration depth and the depth profiles of temperature and its absolute error, after 300 days, are presented.

1. Introduction

Soil freeze-thaw processes play an important role in the engineering design of buildings and constructions, especially on permafrost. The more water-saturated the soil is, the more it is subject to frost heaving, caused by the increase in volume of the soil water, when it turns into ice. A heaving soil may lead to deformation and failure of structures built on it.

Frost penetration into a moist soil implies movement of the water-ice interface dividing the soil into the frozen and unfrozen phase. The mathematical model of heat transfer with a phase transition is a system of partial differential equations with a Stefan condition at the moving boundary of the phase transition. This problem is nonlinear and to solve it, one generally uses numerical methods because an analytical solution is known only for special cases. One of these cases is the Stefan problem of frost penetration into a one-dimensional semi-infinite column of moist soil.

For today, there a lot of software packages for numerical heat transfer. However, not all of them are optimized for solving nonlinear transient heat conduction problems with phase transitions. This feature is important in simulation of seasonal freeze-thaw cycle and thermal effect of buildings and constructions on soil in permafrost areas currently being developed, in particular, for oil and gas production[1],[2],[3],[4].

The purpose of this work is a comparative analysis of the accuracy and speed of solving the soil freezing problem with different software packages. All the numerical solutions are compared with the analytical solution of the well-known Stefan problem of frost penetration[5],[6],[7]. Temperature predictions are made with the software developed in different countries:

- ANSYS Workbench 18.0, Transient Thermal module (USA);
- COMSOL Multiphysics 5.2a (Sweden);
- Frost 3D Universal 3.0 (Russia);
- SV Office 2009, SVHEAT module (Canada);

Note that only Frost 3D and SV Office are positioned as specialized tools for engineering design on permafrost.

2. Problem statement

The problem summary is as follows:

- The calculation area is a semi-infinite ground column (the results up to 25m depth are considered in this problem);
- initial temperature of soil is $T_0 = 1.5$ °C;
- upper boundary is assigned temperature of $T_{bnd} = -27$ °C;
- remaining boundaries are assigned heat flux of $q = 0\ \mathrm{W/m^2}$;
- properties of test soils[8] are given in Table 1;
- volumetric latent heat of freezing of soil water is $L = \rho W_{tot} L_w\ (\mathrm{kJ/m^3})$, where $L_w = 334\ \mathrm{kJ/kg}$ is the latent heat of freezing of water;
- forecast period is 300 days.

Table 1. Properties of test soils

Soil properties	Symbol		Soil				Unit
			Sand		Loam		
	frozen	thawed	frozen	thawed	frozen	thawed	
Thermal conductivity	λ_f	λ_{th}	2.11	1.83	1.64	1.34	$\mathrm{W/(m\cdot °C)}$
Soil density	ρ		1850		1900		$\mathrm{kg/m^3}$
Specific heat capacity	C_f	C_{th}	2.02	2.44	2.05	2.49	$\mathrm{kJ/(kg\cdot °C)}$
Ground freezing point	T_{bf}		-0.05		-0.8		°C
Water content	W_{tot}		0.2		0.175		p.u.

3. Analytical solution of Stefan problem

The classical Stefan problem implies calculation of temperature distribution and phase front tracking in a homogeneous moist soil[15]. It includes the following physical considerations[9]:

1. The phase state (frozen or thawed) of the medium depends on its thermal conductivity and heat capacity.
2. The medium is affected by external heat (cold) sources.
3. In both phases of matter, the energy transfer is governed by the classical heat equation.
4. The behavior of the phase boundary, also known as free boundary, is described by the Stefan condition which expresses the energy balance during the phase transition.
5. In addition to the Stefan condition, there is another condition at the free boundary: the temperature at the boundary surface is equal to the freezing (thawing) point, which is a known constant.

The consideration 5 is an axiomatic statement, because it is not derived from the fundamental laws of thermodynamics, but accurately reflects many real-world processes.

We use the analytical solution (1)–(6) of the classical semi-infinite Stefan problem of frost penetration in z-direction[5]. It is a simple one-dimensional freezing (thawing) problem based on constant boundary and initial conditions. The purpose of the classical Stefan problem solution is to define temperature field and phase boundaries in pure (with no impurities) substance, i.e. - ground[15].

$$T(z,t) = \begin{cases} T_f(z,t), & z < z_{bf}(t) \\ T_{bf}, & z = z_{bf}(t), \\ T_f(z,t), & z > z_{bf}(t) \end{cases} \qquad z_{bf}(t) = \alpha\sqrt{t}, \tag{1}$$

$$T_f(z,t) = T_{bf} + A_f + B_f \operatorname{erf}\left[z/\left(2\sqrt{\lambda_f/C_f\, t}\right)\right], \tag{2}$$

$$T_{th}(z,t) = T_{bf} + A_{th} + B_{th} \operatorname{erf}\left[z/\left(2\sqrt{\lambda_{th}/C_{th}\, t}\right)\right], \tag{3}$$

$$A_f = T_{bnd} - T_{bf}, \qquad B_f = \frac{T_{bf} - T_{bnd}}{\operatorname{erf}\left[\alpha/\left(2\sqrt{\lambda_f/C_f}\right)\right]}, \tag{4}$$

$$A_{th} = \frac{\left(T_{bf} - T_0\right) \operatorname{erf}\left[\alpha/\left(2\sqrt{\lambda_{th}/C_{th}}\right)\right]}{1 - \operatorname{erf}\left[\alpha/\left(2\sqrt{\lambda_{th}/C_{th}}\right)\right]}, \qquad B_{th} = \frac{T_0 - T_{bf}}{1 - \operatorname{erf}\left[\alpha/\left(2\sqrt{\lambda_{th}/C_{th}}\right)\right]}, \tag{5}$$

$$\frac{\lambda_f\left(T_{bnd} - T_{bf}\right)e^{-\alpha^2/(4\lambda_f/C_f)}}{\sqrt{\lambda_f/C_f}\ \operatorname{erf}\left[\alpha/\left(2\sqrt{\lambda_f/C_f}\right)\right]} + \frac{\lambda_{th}\left(T_0 - T_{bf}\right)e^{-\alpha^2/(4\lambda_{th}/C_{th})}}{\sqrt{\lambda_{th}/C_{th}}\ \left(1 - \operatorname{erf}\left[\alpha/\left(2\sqrt{\lambda_{th}/C_{th}}\right)\right]\right)} + \alpha L \frac{\sqrt{\pi}}{2} = 0, \tag{6}$$

where $T(z,t)$ is the temperature at point z and $z_{bf}(t)$ is the frost penetration depth, at time t.

Here (2) and (3) the temperature of frozen and melted ground areas is described. The equations (4) and (5) are coefficients of equations (2) and (3). The solution of the equation (6) derives parameter α, value required for calculation of the equations (4) and (5) coefficients.

4. Numerical solutions in different software packages

ANSYS, COMSOL, Frost 3D, SV Office software packages were used to calculate three-dimensional temperature distribution of thermal field in 300 days, according to Section 2. The solution accuracy was provided by comparison of numerical solution with the classical Stefan problem analytical solution shown in Section 3.

For all software packages it was planned to solve the problem at hexahedron mesh with depth pitch Z of 0.1 meter, and X and Y of 0.5 meter. However, due to particular software features, in COMSOL, SV Office the problem was solved at tetrahedron mesh, and in ANSYS and Frost 3D - at hexahedron mesh (figure 1).

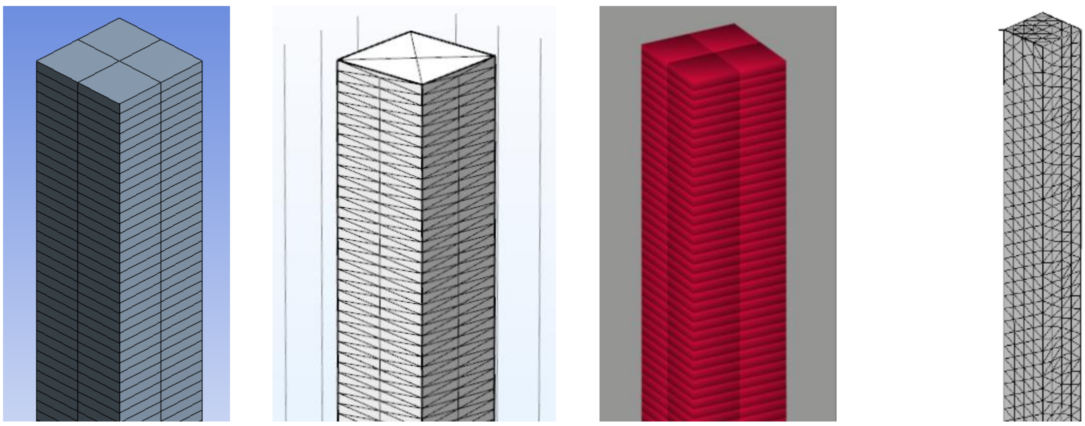

Figure 1. Computation domain meshed in different software packages (left to right): ANSYS, COMSOL, Frost 3D, SV Office

In SV Office it wasn't possible to build the required type mesh, because there are no flexible mesh settings, as in other software packages. For example, in COMSOL, the tetrahedral mesh resembles the rectangular one, because of anisotropic meshing, i.e. direction-dependent mesh density. SV Office yields isotropic meshes only; therefore, the tetrahedral mesh in SV Office is of regularly shaped elements with mesh-size 0.1 m.

In the analytical solution of the classical Stefan problem, the phase transition is sharp, i.e. the soil state at $T \neq T_{bf}$ is either completely frozen or thawed. But when it comes to numerical simulation, one faces the fact that the effective heat capacity has a "virtually infinite" peak[17] at $T = T_{bf}$ In order to handle this, one may (or may not, depending on the kind of software) need to smoothen the phase transition[10]. In that case, the thermal properties of soil are functions of temperature[11], [12], [13]:

$$C_{\text{eff}}(T) = C(T) + L\frac{dw_u}{dT}(T), \qquad L = \rho W_{tot} L_w, \tag{7}$$

$$C(T) = C_f + \left(C_{th} - C_f\right) w_u(T), \tag{8}$$

$$\lambda(T) = \lambda_f + \left(\lambda_{th} - \lambda_f\right) w_u(T), \tag{9}$$

$$w_u(T) = \begin{cases} \dfrac{1}{1 - A\left(T - T_{bf}\right)}, & T < T_{bf} \\ 1, & T \geq T_{bf} \end{cases}, \tag{10}$$

where $C_{\text{eff}}(T)$ is the volumetric effective heat capacity, $C(T)$ is the volumetric heat capacity, $\lambda(T)$ is the thermal conductivity and $w_u(T)$ is the ratio of unfrozen water content at temperature T, A = 10 $^{\circ}$C^{-1} is the sharpness coefficient, which gives a careful smoothing.

All the computations are performed on the Intel Core i5-2500 processor. Solver settings are kept default, were appropriate, in order to test the solution accuracy in the case of minimal user intervention.

4.1. ANSYS Workbench

In ANSYS, to solve a heat transfer problem with phase changes, one should specify material properties in a proper way: enthalpy should be used instead of effective heat capacity or otherwise, the simulation accuracy tends to be too low. The soil enthalpy, as function of temperature, can be derived by integrating the volumetric heat capacity (7) with respect to temperature:

$$H(T) = \int_{-30}^{T} C(\mathrm{T}) d\mathrm{T} + \begin{cases} 0, & T < T_{bf} \\ L, & T \geq T_{bf} \end{cases}. \tag{11}$$

ANSYS allows one to specify material properties as table functions. Hence, we specify the thermal conductivity (9) and enthalpy (11) as table functions of temperature with step of 0.1 °C.

4.2. COMSOL Multiphysics

Unlike ANSYS, COMSOL allows one to specify the effective heat capacity (6) in an explicit way, without loss of simulation accuracy.

COMSOL accepts both table functions and analytical expressions as values of material properties. Therefore, we input the formulas (7)–(10).

4.3. Frost 3D Universal

The formulas (7)–(10) are embedded into Frost 3D, and one has to input the coefficients C_f, C_{th}, λ_f, λ_{th}, T_{bf}, ρ and W_{tot} according to SP 25.13330[8]. Whenever required the user can calculate the

IOP Conf. Series: Materials Science and Engineering **365** (2018) 042059 doi:10.1088/1757-899X/365/4/042059

correlation between heat capacity, thermal conductivity and non-frozen water quantity and input it into software as a table. Correlation input in users formula is not supported by the software.

4.4. SV Office

In the SVHEAT module of SV Office, the heat capacity of soil can be either specified by Jame Newman approach[20],[21] or given constant values for frozen and thawed state. The other temperature-dependent properties of soil can be given table values or an analytical expression. Unfrozen water content specify as a table function of temperature with step of 0.1 °C; the table values are calculated from the formula:

$$\theta(T) = \frac{\rho}{\rho_w} W_{tot} w_u(T), \tag{12}$$

where $\theta(T)$ is the volumetric unfrozen water content, $\rho_w = 1000\ \mathrm{kg/m^3}$ is the water density.

In SV Office time-stepping is non-automatic like in others software packsges and requires manual adjustments. In this case was set initial increment of 1 day and the maximum increment to 10 days.

5. Results

According to the analytical solution (1)–(6) of the Stefan problem, the frost penetration depth after 300 days is 4.21 m for sand and 3.74 m for loam. Comparison of the numerical between analytical solutions is given in figures 2 and 3, and Table 2.

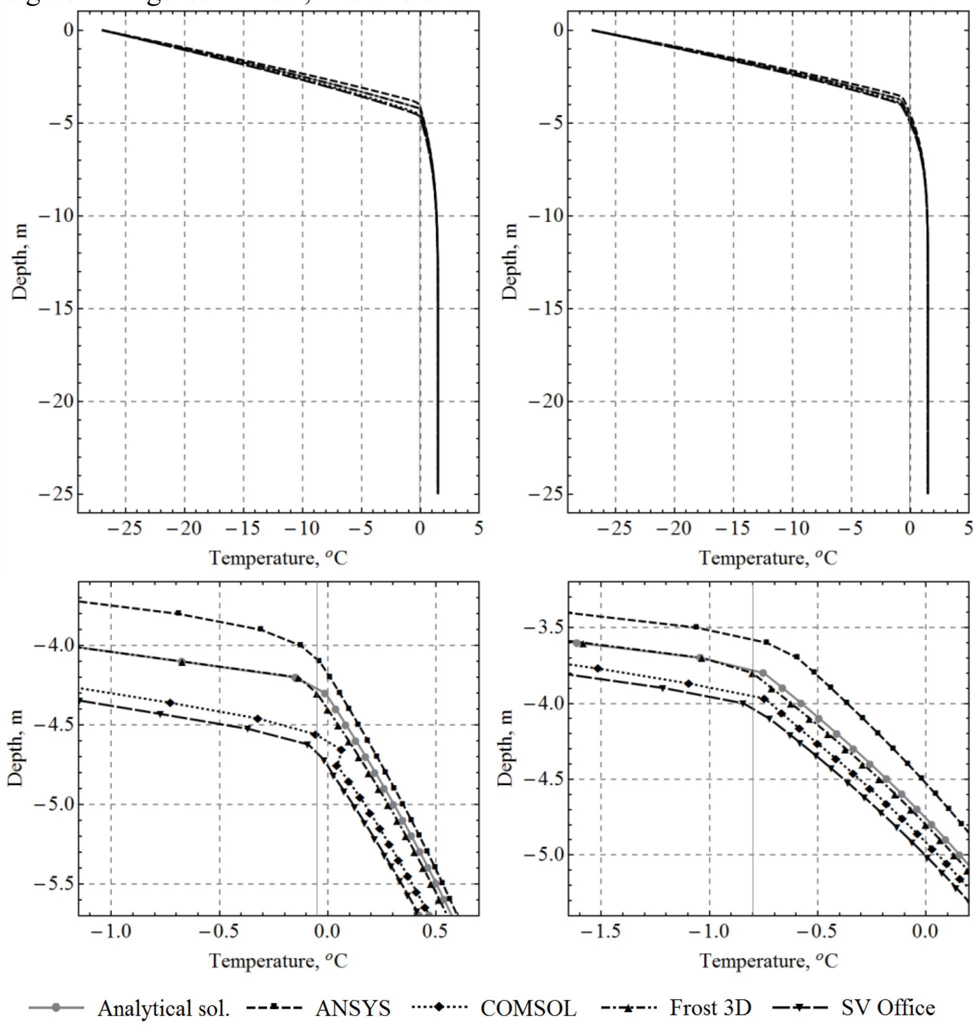

Figure 2. Temperature field after 300 days in loam (left) and sand (right)

In Figure 3 the depth profiles of the absolute error of temperature for all the software packages are presented.

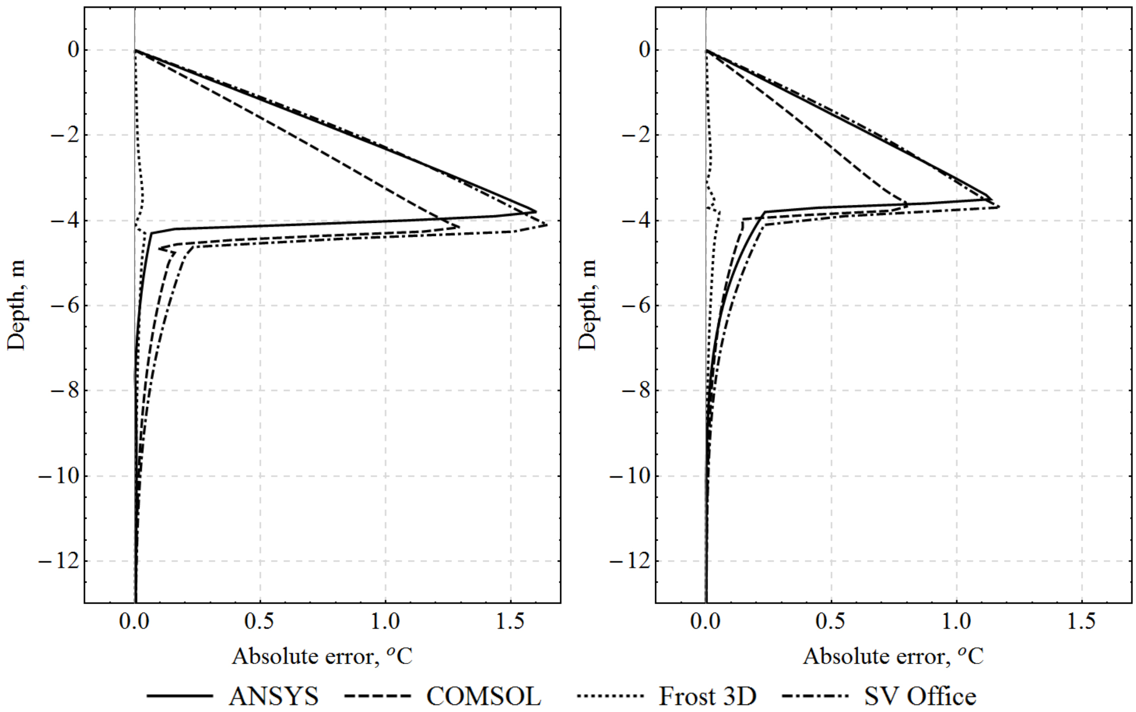

Figure 3. Absolute error in degrees in depth in 300 days in sand (left) and loam (right) in various software packages in comparison with the analytical solution

In Table 2 the max error and running time of all the software packages, as well the frost penetration depth from the analytical and numerical solutions, are provided.

Table 2. Comparison of numerical between analytical solutions of the classical Stefan problem

	Max absolute error (°C)	Max relative error (%)	Frost penetration depth (m)	Time of computation, s
		Loam		
Analytical solution	–	–	3.74	–
SV Office	1.138	3.99	4.02	155[a]
ANSYS	1.134	3.98	3.57	97
COMSOL	0.799	2.81	3.95	280
Frost 3D	0.052	0.18	3.80	7
		Sand		
Analytical solution	–	–	4.21	–
SV Office	1.687	5.92	4.65	178[a]
ANSYS	1.601	5.62	4.08	112
COMSOL	1.295	4.54	4.56	319
Frost 3D	0.039	0.14	4.30	7

[a] Time of computation for a completely different mesh (see Section 4).

All the software packages obtained reasonably good results (max relative error is below 10%) with the max error located near to the phase transition point (see figures 2 and 3). SV Office has the largest error and Frost 3D has the smallest one. Curiously, the solution accuracy for loam was somewhat higher than for sand in all the software packages, except for Frost 3D, and the frost penetration depth was underestimated only by ANSYS. COMSOL has the longest calculation time and Frost 3D has the shortest one, which is much shorter than its nearest competitor (ANSYS) has.

The artifact (non-monotonicity), seen in figure 2, is due to the fact that COMSOL uses the common finite element method. The numerical scheme of the method is different from the well-known monotone finite-difference schemes, even in the case of one-dimensional linear heat transfer: $\frac{dT}{dt}$ is accounted not only in the given node, but in its adjacent nodes, too, in order to approximate $\frac{dT}{dt}$ within finite elements[19]. Moreover, in COMSOL the domain is discetized into an unstructured tetrahedral mesh, and this may worsen the situation, too[18]. Note, that the artifact is predictably located at the phase boundary, where the nonlinearity of the problem is the stongest.

The solution accuracy by absolute error in SV Office is almost the same as in ANSYS. But calculation time in ANSYS is over 1.5 times longer than in SV Office where the higher number of mesh elements.

Such different computational results can be explained by differences in the used numerical methods and their default settings for solving the nonlinear Stefan problem with a moving boundary of the phase transition. ANSYS, COMSOL and SV Office is based on implicit formulation of the finite-element method, with a problem of convergence of numerical method for solving 3D problems. Frost 3D is based on explicit formulation of the finite-difference scheme that is the best solution for the considered problem in 3D.

6. Summary

Comparison of the numerical results, obtained by such software as ANSYS Workbench 18.0 (Transient Thermal module), COMSOL Multiphysics 5.2a, Frost 3D Universal 3.0, SV Office 2009 (SVHEAT module), with the analytical solution of the Stefan problem was considered. The comparison showed that Frost 3D has the better convergence with the analytical solution (max relative error of 0.18% for loam) and calculation time (7 s). Good results were shown by COMSOL (max 4.54%), ANSYS (max 5.62%) and SV Office (max 5.96%), but the ANSYS results underestimates the frost penetration depth, which is important for construction engineering in permafrost regions, and COMSOL computational time was greater (max 319 s.), in comparison with other software packages.

References

[1] Oswell J M and Nixon J F 2015 Thermal Design Considerations for Raised Structures on Permafrost *Journal of Cold Regions Engineering* V29 Issue 1

[2] Zhou F Li R, Zhang A and Zhu L 2008 Surface-coupled three-dimensional geothermal model for study of permafrost geothermal regime in a building environment *Journal of Geophysical Research: Atmospheres* V113 Issue D19

[3] Gishkeluk I A, Stanilovskaya J V and Evlanov D V 2015 Forecasting of permafrost thawing around an underground cross-country pipeline *Oil & Oil products pipeline transportation: Science & Technologies №1* V17 pp 20–25

[4] Kudriavtcev S, Valtseva T, Kazharskyi A, Goncharova E and Berestianyi I 2013 Predictive modeling of the permafrost thermal regime in Russian railroad subgrade support systems *Journal of Sciences in Cold and Arid Regions* V4(5) pp 404-407

[5] Pavlova AR 2001 *Mathematical modeling of heat and mass transfer processes during phase transitions* (Yakutsk – Tutorial) p.55

[6] Boucígueza A C, Lozanoa R F and Larab M A, 2007. About the exact solution in two-phase Stefan problem *Journal of Thermal Engineering* V6 pp 70-75

[7] Javierre E, Vuik C, Vermolen F J and van der Zwaag S 2006 A comparison of numerical models for one-dimensional Stefan problems *Journal of Computational and Applied Mathematics* V192 pp 445 – 459
[8] SP 25.13330.2012 *Soil bases and foundations on permafrost soils. The updated edition SNiP 2.02.04-88*
[9] J Stefan 1889 *Über einige Probleme der Theorie der Warmeleitung* (S. Ber. Wieh. Akad. Mat. Natur) V98 pp. 473-484.
[10] Anisimov O A 2012 *Methods for assessing the effects of climate change on physical and biological systems* Chapter 8. Continental permafrost (Roshydromet) p 508
[11] Kudryavtsev S A 2004 *Geotechnical modeling of the process of freezing and deterioring of frozen soils* (Moscow: ACB Article) p 36
[12] Kazarnovsky V D, Grechishchev S E and etc, 2003 *Methodical recommendations for the use of large-diameter metal pipes in conditions of icing and permafrost soils*
[13] Tsytovich N A 1973 *Mechanics of frozen soils* (Moscow: High school – Tutorial) p.448
[14] Nagornova T A 2005 Mathematical modeling of the freezing process of moisture saturated soil *Journal Proceedings of TPU* (Tomsk) p.127-128
[15] Lykov A V 1967 *Theory of heat conductivity* (Moscow: High school – Tutorial) p.599
[16] Kudryavtsev S A 2004 Calculation of the process of freezing and throwing by the program Termoground *Journal Reconstruction of cities and geotechnical construction* (Saint Petersburg) pp 83-97
[17] Feulvarch E Roux J-C and Bergheau J-M 2013 Theoretical Framework of a Variational Formulation for Nonlinear Heat Transfer with Phase Changes *Journal Mathematical Problems in Engineering* V2013 p. 6
[18] Lipnikova K, Shashkova M, Svyatskiya D and Vassilevskib Yu 2007 Monotone finite volume schemes for diffusion equations on unstructured triangular and shape-regular polygonal meshes *Journal of Computational Physics* V227 Issue 1 pp 492-512
[19] Emery A F and Mortazavi H R 1982 A comparison of the finite difference and finite element methods for heat transfer calculations *Proceedings of a Joint NASA/George Washington University/Old Dominion University Symposium* V1 pp 51-82
[20] Jame Y W 1977 Heat and mass transfer in freezing unsaturated soil *PhD Dissertation,* (University of Saskatchewan) p 212
[21] Newman G and Wilson G 1997 Heat and mass transfer in unsaturated soils during freezing. *Canadian Geotechnical Journal* V34 pp 63-70