MIKE
Powered by DHI

piFreeze

A Freeze / Thaw Plug-in for FEFLOW

User Guide

DHI headquarters
Agern Allé 5
DK-2970 Hørsholm
Denmark

+45 4516 9200 Telephone
+45 4516 9333 Support
+45 4516 9292 Telefax

mike@dhigroup.com
www.mikepoweredbydhi.com

CONTENTS

piFreeze
A Freeze / Thaw Plug-in for FEFLOW
User Guide

1 Introduction 1

2 Installation 1

3 Licence file and dongle 1

4 Product invocation 1

5 Product usage 2

6 Theoretical background 3
6.1 Introduction 3
6.2 Ice phase 3
6.2.1 Modification of unsaturated flow equation 5
6.2.2 Modification of heat transport equation 6
6.3 Validation and tests 7
6.3.1 Frozen wall problem 7
6.4 References 11

7 Support 12

1 Introduction

Phase changes from water to ice and vice versa occur in natural groundwater systems and due to human activity. Through latent heat, influencing the effective hydraulic conductivity and affecting the thermal properties they have a major influence on both fluid flow and the temperature regime. In many practical application cases it is thus not safe to ignore them.

FEFLOW piFreeze, a plug-in to FEFLOW, supports the convenient extension of any two- or three-dimensional FEFLOW flow and transport models using Richards' equation by phase changes between water and ice.

2 Installation

To install FEFLOW piFreeze, you have two different options:

- For the plug-in to work with the 32-bit version of FEFLOW, copy all the FEFLOW piFreeze files except piFreeze_x86.dll into C:\Program Files\DHI\2016\FEFLOW 7.0\modules32.
- For the plug-in to work with the 64-bit version of FEFLOW, copy all the FEFLOW piFreeze files except piFreeze_x64.dll into C:\Program Files\DHI\2016\FEFLOW 7.0\modules64.

You may do both, of course.

Alternatively, you may store the plug-in files in any location and use the Register Plug-in button in the FEFLOW Plug-ins panel to add piFreeze to the list of available plug-ins.

3 Licence file and dongle

piFreeze requires a licence separate from your FEFLOW licence. The software licence can be retrieved through your local office.

To install the licence, please follow the installation guidelines provided with the installation.

4 Product invocation

To load piFreeze to the current FEFLOW model, double click on the piFreeze entry in the Plug-ins panel in FEFLOW or choose Attach from its context menu.

Please note that piFreeze can only be added to models using Richards' equation (unsaturated or variably saturated media). This setting is done on the Problem Class page of the Problem Settings dialogue in FEFLOW.

5 Product usage

The piFreeze plug-in is applied once it is attached to the current FEFLOW model, and as long as it is not deactivated by unchecking the checkbox in front of its name. Unchecking, in comparison with detaching piFreeze, has the advantage that potential custom parameters that have been defined are kept.

The piFreeze parameter dialogue is opened by either choosing Activate from its context menu or by hitting the Edit button of the plug-ins panel.

The following parameters can be defined (values indicate defaults):

Liquid density	1000	kg/m^3	Density of the fluid phase
Ice density	917.5	kg/m^3	Density of the ice phase
Ice heat capacity	1860000	J/m^3 K	Volumetric heat capacity of the ice phase
Ice thermal conductivity	190080	J/(mdK)	Thermal conductivity of the ice phase
Latent heat	334000	J/K	Enthalpy of fusion
Freezing temperature	0	°C	Freezing temperature (centre point of freezing interval)
Half of delta temperature	1	°C	Freezing interval is from Freezing temperature + Half of delta temperature to Freezing temperature - Half of delta temperature. The freezing function is assumed as linear within the interval.
Residual liquid fraction	0.0001	-	Residual fraction of the liquid phase. Required to avoid a reduction of hydraulic conductivity to zero.

User-defined parameters are stored with the FEFLOW model in the *.fem and *.dac files.

6 Theoretical background

6.1 Introduction

FEFLOW groundwater modelling software [1] is capable to simulate unsaturated flow including mass and heat transport processes. But the heat transport doesn't take into account freezing of groundwater that is a natural process in northern countries. The groundwater freezing can also be applied technically in mining processes.

The new FEFLOW **FreezeThaw** plug-in extends the heat transport in unsaturated flow modelling with the freezing and thawing of water depending on the temperature.

6.2 Ice phase

Additionally to the three phases: *air*, *liquid* and *solid* of partially saturated flow, the new phase *ice* is introduced. The volumetric bulk fraction of the corresponding phase is denoted as ε_a, ε_l, ε_s and the additional ε_i. By definition, the sum of fractions equals 1:

$$\varepsilon_a + \varepsilon_l + \varepsilon_s + \varepsilon_i = 1. \tag{1}$$

The pore space available for the fluid flow is $\varepsilon = \varepsilon_a + \varepsilon_l$ and called *porosity* in FEFLOW. The relation of the liquid fraction to the pore space $s = \varepsilon_l/\varepsilon$ is *saturation*. To establish a relation between ice and liquid, we introduce the mass fraction per bulk volume of the unfrozen liquid to the total liquid mass:

$$\varphi = \frac{\varepsilon_l \rho_l}{\varepsilon_l \rho_l + \varepsilon_i \rho_i}, \tag{2}$$

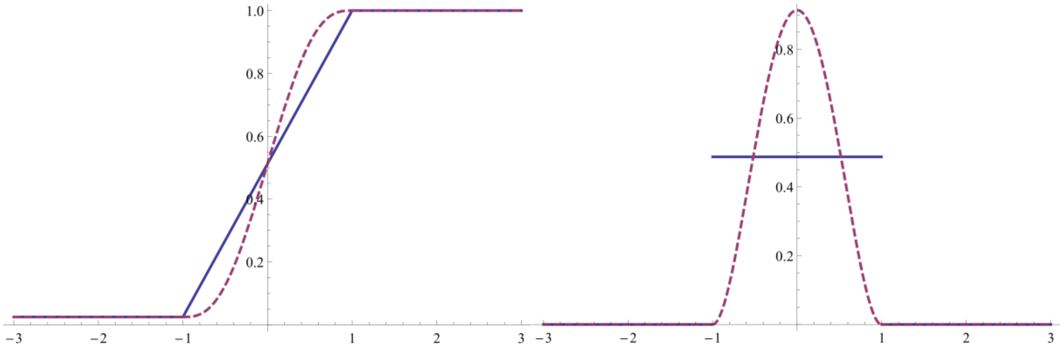
where $\rho_x,\ x \in \{a, l, s, i\}$ is the density of the corresponding phase. The function φ is also known as the freezing function, decreasing, however, with the fraction of ice. When the freezing point is T_0, then the ice doesn't appear immediately for temperatures below T_0, but forms gradually withing the predefined temperature interval $[T_l, T_h] = [T_0 - \frac{\Delta T}{2}, T_0 + \frac{\Delta T}{2}]$ of the length ΔT. Even below this interval, some liquid fraction φ_{res} can always remain mobile. The simplest shape of the function φ fullfiling the described freezing behavior is the linear one in the interval $[T_l, T_h]$ with the constant continuation outside of the interval (Figure 1, solid line)

$$\varphi(T) = \begin{cases} \varphi_{\text{res}}, & T < T_l, \\ \varphi_{\text{res}} + (1 - \varphi_{\text{res}}) \dfrac{T - T_l}{\Delta T}, & T_l \le T < T_h, \\ 1, & T \ge T_h. \end{cases} \tag{3}$$

The first derivative $\frac{\partial \varphi}{\partial T}$ is a step function. A smooth version of it applies a polynomial of the fifth order (Figure 1, dashed line)

$$\varphi(T) = \begin{cases} \varphi_{\text{res}}, & T < T_l, \\ \varphi_{\text{res}} + (1 - \varphi_{\text{res}}) \tilde{T}^3 \left(6\tilde{T}^2 - 15\tilde{T} + 10\right), & T_l \le T < T_h, \\ 1, & T \ge T_h, \end{cases} \tag{4}$$

where $\tilde{T} = \frac{1}{\Delta T}\left(T + \frac{\Delta T}{2}\right)$.



a) Function φ b) Derivative $\frac{\partial \varphi}{\partial T}$

Figure 1 Freezing function φ (a) and its derivative (b) with parameters Δt = φ_{res} =0.025

Since ice occupies bigger volume than the liquid it was created from, there are two different assumptions depending on states of the porous media during ice formation:

1. Partially saturated state: $\varepsilon_a > 0,\ s < 1$. It is assumed that expansion from freezing happens locally into space occupied by air phase. In this case no water mass is transferred across REV boundary and local water mass remains constant

$$\varepsilon_l \rho_l + \varepsilon_i \rho_i = \text{const.} \tag{5}$$

   The bulk volume fractions for liquid and ice can be then expressed over φ

$$\begin{aligned} \varepsilon_l &= \frac{\varphi(\varepsilon_l \rho_l + \varepsilon_i \rho_i)}{\rho_l} = \varphi\left(\varepsilon_l + \varepsilon_i \frac{\rho_i}{\rho_l}\right), \\ \varepsilon_i &= \frac{(1-\varphi)(\varepsilon_l \rho_l + \varepsilon_i \rho_i)}{\rho_i} = (1-\varphi)\left(\varepsilon_l \frac{\rho_l}{\rho_i} + \varepsilon_i\right). \end{aligned} \tag{6}$$

   The corresponding derivatives with respect to φ are

$$\frac{\partial \varepsilon_l}{\partial \varphi} = \varepsilon_l + \varepsilon_i \frac{\rho_i}{\rho_l}, \qquad \frac{\partial \varepsilon_i}{\partial \varphi} = -\varepsilon_i - \varepsilon_l \frac{\rho_l}{\rho_i}. \tag{7}$$

2. Fully saturated state: $\varepsilon_a = 0,\ s = 1$. If no air is present, expansion from freezing will displace water mass as total available space is then fixed

$$\varepsilon_l + \varepsilon_i = 1 - \varepsilon_s = \text{const.} \tag{8}$$

   The bulk volume fractions for liquid and ice are then expressed over φ as follows

$$\begin{aligned} \varepsilon_l &= \frac{\varphi(\varepsilon_l + \varepsilon_i)\rho_i}{\rho_l + \varphi\rho_i - \varphi\rho_l} = \frac{\varphi(\varepsilon_l + \varepsilon_i)\frac{\rho_i}{\rho_l}}{1 - \varphi\left(1 - \frac{\rho_i}{\rho_l}\right)}, \\ \varepsilon_i &= \frac{(1-\varphi)(\varepsilon_l + \varepsilon_i)\rho_l}{\rho_l + \varphi\rho_i - \varphi\rho_l} = \frac{(1-\varphi)(\varepsilon_l + \varepsilon_i)}{1 - \varphi\left(1 - \frac{\rho_i}{\rho_l}\right)}. \end{aligned} \tag{9}$$

The corresponding derivatives with respect to φ are

$$\frac{\partial \varepsilon_l}{\partial \varphi} = \frac{(\varepsilon_l + \varepsilon_i)\frac{\rho_i}{\rho_l}}{\left[1 - \varphi\left(1 - \frac{\rho_i}{\rho_l}\right)\right]^2}, \qquad \frac{\partial \varepsilon_i}{\partial \varphi} = -\frac{(\varepsilon_l + \varepsilon_i)\frac{\rho_i}{\rho_l}}{\left[1 - \varphi\left(1 - \frac{\rho_i}{\rho_l}\right)\right]^2}. \tag{10}$$

6.2.1 Modification of unsaturated flow equation

Ice phase described by its bulk volumetric fraction ε_i is unknown to FEFLOW. It is, therefore, needed to modify flow and heat parameters during ice formation ($\varepsilon_i > 0$). FEFLOW's porosity $\varepsilon = \varepsilon_a + \varepsilon_l$ is the pore space of the total volume, while the ice fraction decreases the pore space and belongs to the solid part of the porous media. As follows, the ice fraction ε_i must be subtracted from the initial porosity ε_0.

As assumed above, the ice formation in a partially saturated state will occupy air space, which is also accounted within the porosity ε. The relative conductivity is also variable depending on saturation. FEFLOW provides five empirical models and cubic splines to define the saturation on pressure and the relative conductivity on saturation dependencies. Due to ice formation, the relative conductivity goes down linearly up to the small non-zero residual value, e.g. $k_{\text{res}} = 10^{-6}$, :

$$k_r(T) = \begin{cases} k_{\text{res}}, & T < T_l, \\ k_{\text{res}} \quad + (1 - k_{\text{res}})\dfrac{T - T_l}{\Delta T}, & T_l \le T < T_h, \\ 1, & T \ge T_h. \end{cases} \tag{11}$$

In a fully saturated state, a volumetric source/sink contribution Q_f should also be taken into account. To derive it, we consider the mass conservation of ice phase first:

$$\frac{\partial(\varepsilon_i \rho_i)}{\partial t} = R_i - \nabla \cdot (v_s \varepsilon_i \rho_i), \tag{12}$$

where R_i is the rate of the creation of ice mass per bulk volume. The solid velocity v_s is assumed to be zero. Since the density ρ_i is the constant over time, the mass conservation of ice reduces to

$$\rho_i \frac{\partial \varepsilon_i}{\partial t} = R_i. \tag{13}$$

The rate R_i should come as an additional sink term into the right side of the Richards equation:

$$S_0 \rho_l s(h)\left(\frac{\partial h}{\partial t} + \frac{\partial(\varepsilon_l \rho_l)}{\partial t}\right) + \nabla \cdot (\rho_l \boldsymbol{q}) = Q - R_i \tag{14}$$

Introducing the freezing function φ and assuming a constant ρ_l and $Q = 0$, the latter equation can be developed to

$$S_0 s(h)\frac{\partial h}{\partial t} + \varepsilon\left(\frac{\partial s}{\partial h}\frac{\partial h}{\partial t} + \frac{\partial s}{\partial \varphi}\frac{\partial \varphi}{\partial t}\right) + s\frac{\partial \varepsilon}{\partial \varphi}\frac{\partial \varphi}{\partial t} + \nabla \cdot \boldsymbol{q} = \frac{\rho_i}{\rho_l}\frac{\partial \varepsilon_i}{\partial \varphi}\frac{\partial \varphi}{\partial t}. \tag{15}$$

Assuming that $\frac{\partial s}{\partial \varphi} = 0$ and moving all the terms with the function φ to the right side forms it into the target sink term

$$Q_f = -\frac{\partial \varphi}{\partial t}\left[\frac{\rho_i}{\rho_l}\frac{\partial \varepsilon_i}{\partial \varphi} + s\frac{\partial \varepsilon}{\partial \varphi}\right] = -\frac{\partial \varphi}{\partial T}\frac{\partial T}{\partial t}\left[\frac{\rho_i}{\rho_l}\frac{\partial \varepsilon_i}{\partial \varphi} + \frac{\partial \varepsilon_l}{\partial \varphi}\right]. \tag{16}$$

6.2.2 Modification of heat transport equation

The ice fraction can be seen as a second solid phase with its own properties including thermal conductivity and capacity. The bulk thermal conductivity λ for an unsaturated flow is computed in FEFLOW internally as

$$\lambda = \epsilon s \lambda_l + (1 - \varepsilon)\lambda_s = \varepsilon_l \lambda_l + \varepsilon_s \lambda_s, \tag{17}$$

where liquid water and solid matrix conductivities λ_l and λ_s can be read and set over IFM functions. In the presence of ice, the bulk thermal conductivity receives a term with the ice conductivity and becomes

$$\lambda = \varepsilon_l \lambda_l + \varepsilon_s \lambda_s + \varepsilon_i \lambda_i, \tag{18}$$

To substitute the proper conductivity ([e12]) in FEFLOW having access to λ_l or λ_s only, the liquid conductivity can remain unchanged and the solid conductivity should be modified with respect to the initial value to

$$\lambda_s = \lambda_{s,0} + \frac{\varepsilon_i(\lambda_i - \lambda_s)}{1 - \varepsilon}. \tag{19}$$

Similar is the calculation of the volumetric heat capacity

$$C = \varepsilon s C_l + (1 - \varepsilon)C_s = \varepsilon_l C_l + \varepsilon_s C_s, \tag{20}$$

which in presence of ice becomes

$$C = \varepsilon_l C_l + \varepsilon_s C_s + \varepsilon_i C_i - \rho_i L_f \frac{\partial \varepsilon_i}{\partial \varphi}\frac{\partial \varphi}{\partial T}, \tag{21}$$

where L_f is the latent heat of the ice formation. To set the proper volumetric heat capacity in FEFLOW access to C_l or C_s only, the liquid capacity can remain unchanged and the solid capacity should be modified with respect to the initial value to

$$C_s = C_{s,0} + \frac{\varepsilon_i(C_i - C_s)}{1 - \varepsilon} - \frac{\rho_i L_f}{1 - \varepsilon}\frac{\partial \varepsilon_i}{\partial \varphi}\frac{\partial \varphi}{\partial T}. \tag{22}$$

6.3 Validation and tests

6.3.1 Frozen wall problem

This problem is a fully saturated flow through a simple rectangular domain of porous media in presence of a thin wall with a constant temperature below freezing point (zero) described in Figure 2, cf. Ref. /2/. The fluid flow is induced by the pressure difference between left and right boundary. The pressure is set as a fixed Dirichlet boundary condition and is 500 Pa higher on the left boundary. The temperature Dirichlet boundary condition is set on the left boundary to $5°\mathrm{C}$ and on the wall to $-5°\mathrm{C}$. The initial temperature equals $5°\mathrm{C}$ everywhere. The model is discretized by a uniform rectangular grid with a step size of 0.5 m. The freezing function φ is linear with $\Delta T = 2$ and $\varphi_{\mathrm{res}} = 0.025$. The simulation length is set to 800 days during that the model comes into an equilibrium state. Adaptive time step predictor-corrector scheme is used for time discretization.

The material parameters summarized in Table 1 have been taken from, where the same model was computed using SUTRA-ICE software. The only difference in the parameters is the presence of gravity in FEFLOW that cannot be switched off in an unsaturated flow model, but may lead to results variation, since the difference in the pressure that drives the flow is moderate. Figure 4 shows the time development of the simulation at six time points. The colour field reflects the temperature distribution, the vectors in mesh nodes indicate the direction and the magnitude of the velocity field.

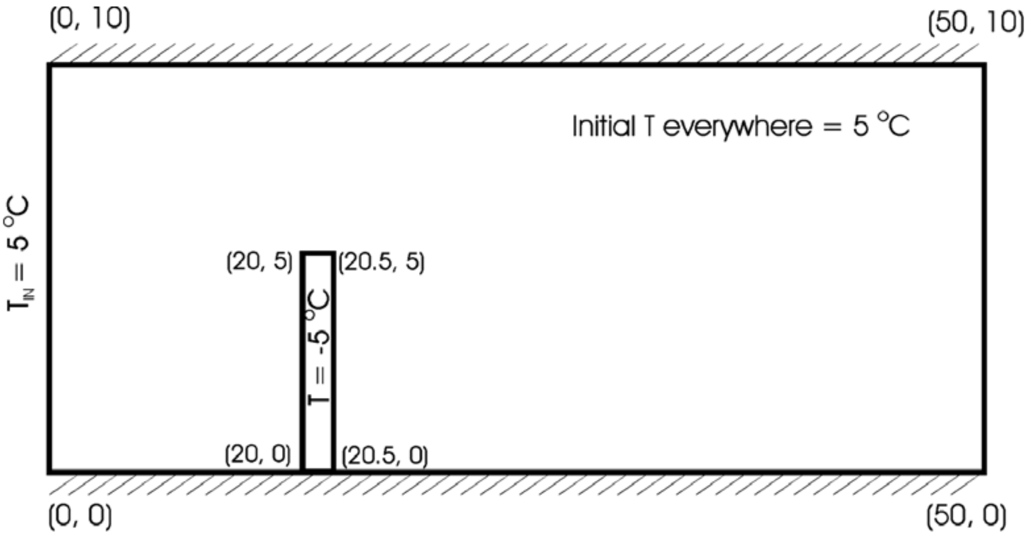


Figure 2 Frozen wall problem description

Table 1 Model parameters for the frozen wall test

Parameter	Unit	Value
Gravity	$\left[\frac{m}{s^2}\right]$	-9.81
Porosity	[]	0.1
Saturated conductivity	$\left[\frac{m}{s}\right]$	0.0011
Specific storage (compressibility)	$\left[\frac{1}{m}\right]$	0
Fluid thermal conductivity	$\left[\frac{J}{msK}\right]$	0.6
[1mm] Solid thermal conductivity	$\left[\frac{J}{msK}\right]$	3.5
[1mm] Ice thermal conductivity	$\left[\frac{J}{msK}\right]$	2.14
[1mm] Fluid volumetric heat capacity	$\left[\frac{J}{m^3K}\right]$	4182000
[1mm] Solid volumetric heat capacity	$\left[\frac{J}{m^3K}\right]$	1939360
[1mm] Ice volumetric heat capacity	$\left[\frac{J}{m^3K}\right]$	2184000
[1mm] Latent heat of fusion	$\left[\frac{J}{kg}\right]$	334000
Longitudinal dispersivity	$[m]$	5
Transverse dispersivity	$[m]$	0.5

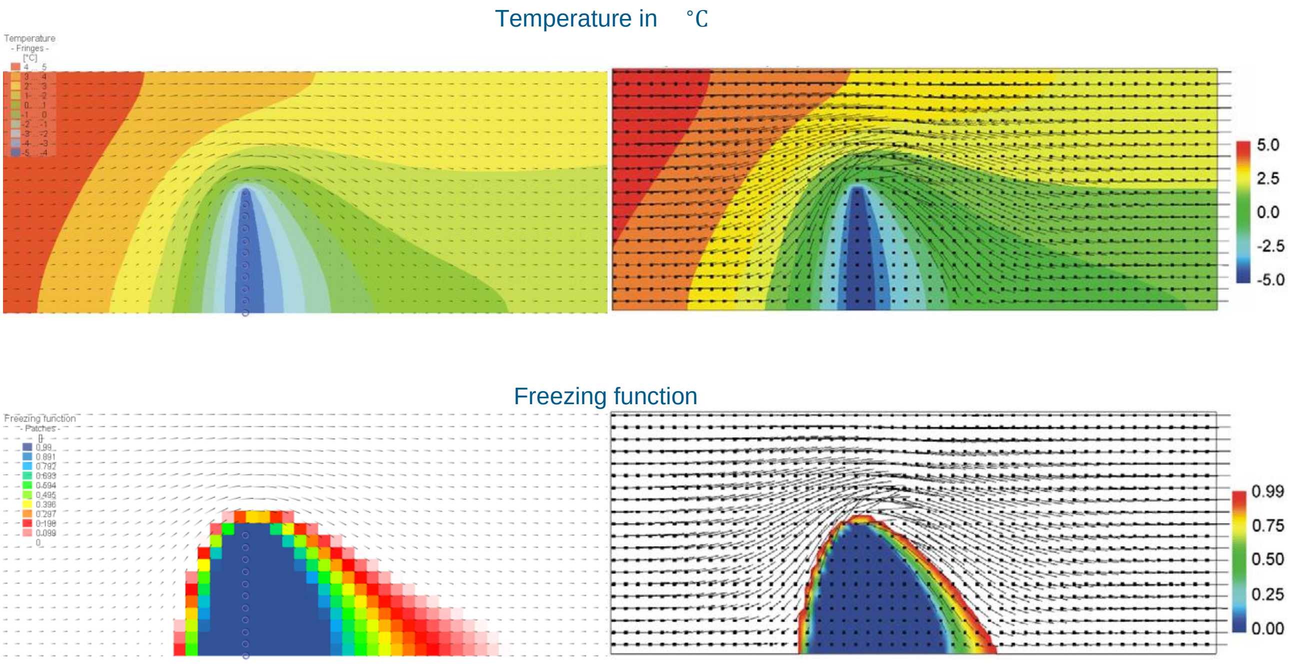


Figure 3 Temperature distribution and velocity vectors comparison of FEFLOW (left) vs. SUTRA-ICE (Ref. /[2/) at 800 days. Both FEFLOW and SUTRA-ICE apply linear freezing (3) and conductivity (11) relations on the same numerical mesh

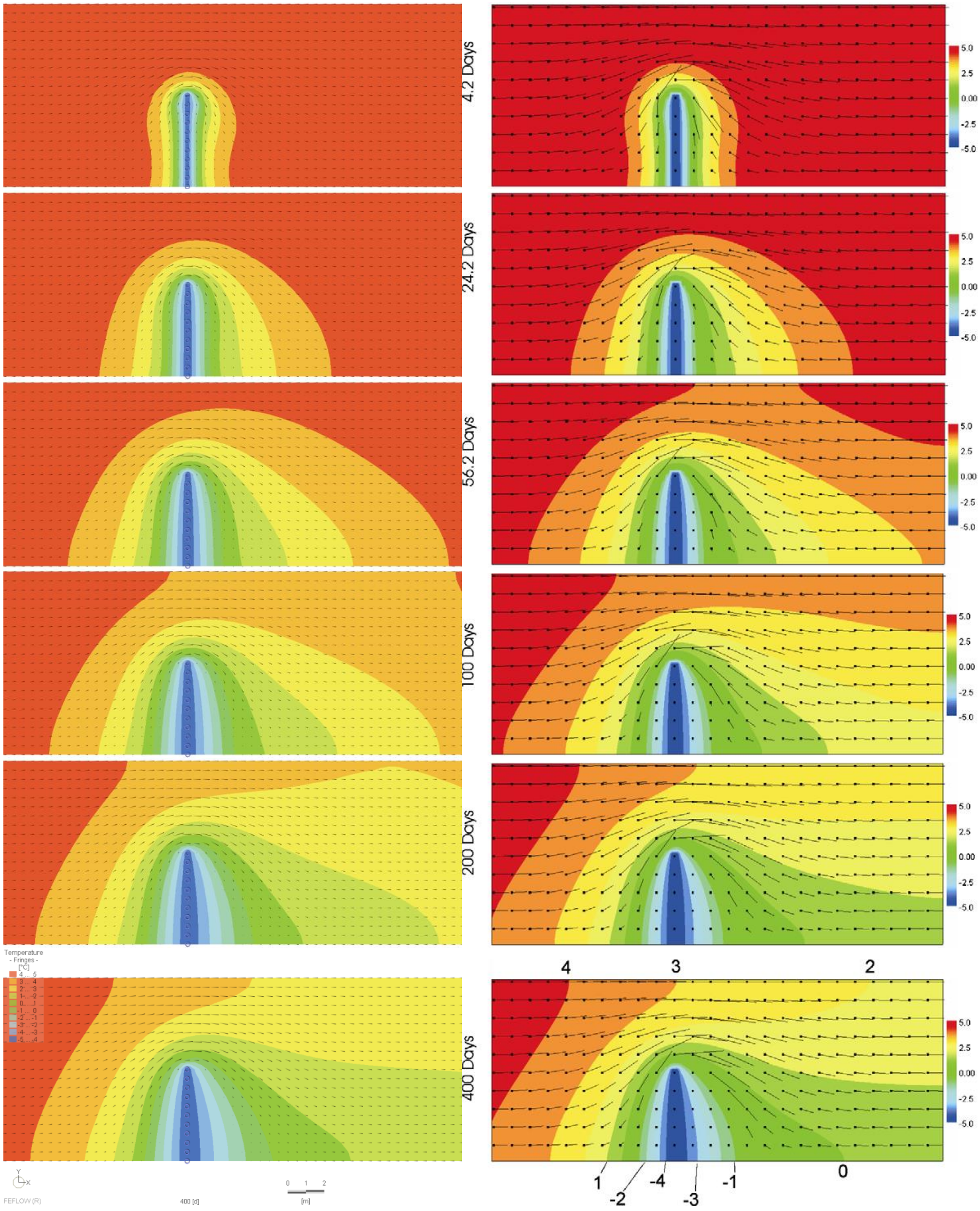


Figure 4 Temperature distribution and velocity vectors comparison of FEFLOW (left) vs. SUTRA-ICE (Ref. /2/) over time. FEFLOW applies linear freezing (3) and conductivity (11) relations. SUTRA-ICE results correspond to exponential freezing and conductivity relations. FEFLOW numerical mesh is double as fine.

6.4 References

/1/ Diersch, Hans-Jörg. FEFLOW. *Finite element modeling of flow, mass and heat transport in porous and fractured media*. Springer, Berlin, 2014.

/2/ J. M. McKenzie, C. I. Voss, and D. I. Siegel. *Groundwater flow with energy transport and waterice phase change: Numerical simulations, benchmarks, and application to freezing in peat bogs*. Advances in Water Resources, 30(4):966 - 983, 2007.

7 Support

If you experience any difficulties, or if you have any questions, you can contact Client Care by mail, e-mail, phone or fax:

MIKE Powered by DHI Client Care
DHI
Agern Allé 5
DK-2970 Hørsholm
Denmark

+45 4516 9333 Telephone
+45 4516 9292 Telefax
mike@dhigroup.com
http://www.mikepoweredbydhi.com/

Or you can find your local Client Care with support in your local language here.