



Phase Change in a Semi-Infinite Soil Column

Introduction

The freezing of subsurface water has a high impact on groundwater flow and subsurface heat transfer. This example models the freezing of a soil column over time. This is a benchmark model as an analytical solution (Lunardini, 1985) exists.

Lunardini developed an exact analytical solution for the propagation of subfreezing temperatures in a semi-infinite, initially unfrozen porous medium with time. He therefore divided the porous medium in three zones: A totally frozen zone (for temperatures $T < T_m$), a so-called mushy or partially frozen zone ($T_m < T < T_f$), and a totally unfrozen or liquid water zone ($T > T_f$).

This example uses the **Phase Change Material** subfeature from the **Heat Transfer in Porous Media** interface.

This example demonstrates how to model a phase change between water and ice using a user-defined phase transition function. The solution should be equal to that of Lunardini.

Model Definition

In this example, the soil column is approximated by a line interval of 10 m length. The initial temperature is 4°C and the temperature at one end is set to -6°C while the other end is thermally isolated.

The following equation is solved:

$$(\rho C_p)_{\text{eff}} \frac{\partial T}{\partial t} + \nabla \cdot (-k_{\text{eff}} \nabla T) = Q \quad (1)$$

Here, T is the temperature (K) and Q is a heat source (W/m^3). The effective values are defined as

$$(\rho C)_{\text{eff}} = \varepsilon_p \rho_f C_{p,f} + \theta_s \rho_s C_{p,s} + \theta_{\text{imf}} \rho_{\text{imf}} C_{p,\text{imf}} \quad (2)$$

$$k_{\text{eff}} = \varepsilon_p k_f + \theta_s k_s + \theta_{\text{imf}} k_{\text{imf}} + k_{\text{disp}} \quad (3)$$

where ρ (kg/m^3) is the density (of the fluid, solid, and immobile fluid), C_p ($\text{J}/(\text{kg}\cdot\text{K})$) the heat capacity at constant pressure, and k the thermal conductivity ($\text{W}/(\text{m}\cdot\text{K})$).

Results and Discussion

Figure 1 shows the temperature profile after 24, 48, and 72 h and compares the computed results (solid line) with the analytical solution provided in Ref. 1.

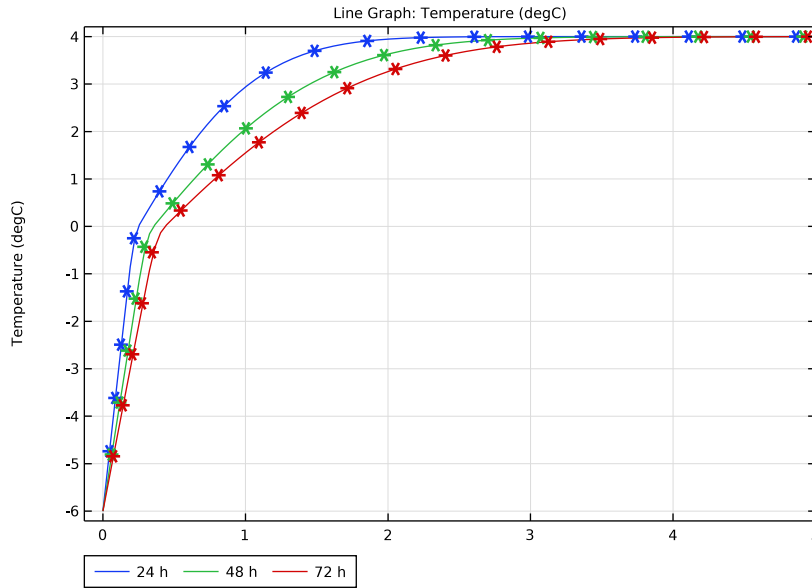


Figure 1: Computed (solid line) compared to analytical solution (asterisks) after 24, 48, and 72 h.

The results match very well.

References

1. https://wiki.lsce.ipsl.fr/interfrost/doku.php?id=test_cases:one.
2. C. Grenier, D. Régnier, E. Mouche, H. Benabderrahmane, F. Costard, and P. Davy, "Impact of permafrost development on underground flow patterns: a numerical study considering freezing cycles on a two dimensional vertical cut through a generic river-plain system," *Hydrogeology Journal*, vol. 21, no. 1, pp. 257–270, 2013.

Application Library path: Porous_Media_Flow_Module/Verification_Examples/
phase_change_lunardini

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click  **Model Wizard**.

MODEL WIZARD

- 1 In the **Model Wizard** window, click  **1D**.
- 2 In the **Select Physics** tree, select **Heat Transfer>Porous Media>Heat Transfer in Porous Media (ht)**.
- 3 Click **Add**.
- 4 Click  **Study**.
- 5 In the **Select Study** tree, select **General Studies>Time Dependent**.
- 6 Click  **Done**.

GEOMETRY 1

Interval 1 (il)

The model domain is approximated by a 1D line segment of 10 m length.

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Geometry 1** and choose **Interval**.
- 2 In the **Settings** window for **Interval**, locate the **Interval** section.
- 3 In the table, enter the following settings:

Coordinates (m)
0
10

- 4 Click  **Build All Objects**.

GLOBAL DEFINITIONS

Now, enter the parameters used in the model. You can import them from an external file.

Parameters 1

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `phase_change_Lunardini_parameters.txt`.

HEAT TRANSFER IN POROUS MEDIA (HT)

Follow the steps below to set up the physics.

Fluid 1

In the **Model Builder** window, expand the **Component 1 (comp1)>**

Heat Transfer in Porous Media (ht)>Porous Medium 1>Fluid 1 node, then click **Fluid 1**.

Phase Change Material 1

- 1 In the **Physics** toolbar, click  **Attributes** and choose **Phase Change Material**.
- 2 In the **Settings** window for **Phase Change Material**, locate the **Phase Change** section.
- 3 From the **Phase transition function** list, choose **User defined**. In the $L_{1 \rightarrow 2}$ text field, type `L`.
- 4 In the $\alpha_{1 \rightarrow 2}$ text field, type `f_phtn(T)`, which is yet to be defined.
- 5 Locate the **Phase 1** section. From the k_1 list, choose **User defined**. In the associated text field, type `k_ice`.
- 6 From the ρ_1 list, choose **User defined**. In the associated text field, type `rho_ice`.
- 7 From the $C_{p,1}$ list, choose **User defined**. In the associated text field, type `Cv/rho_ice`.
- 8 Locate the **Phase 2** section. From the k_2 list, choose **User defined**. In the associated text field, type `k_water`.
- 9 From the ρ_2 list, choose **User defined**. In the associated text field, type `rho_water`.
- 10 From the $C_{p,2}$ list, choose **User defined**. In the associated text field, type `Cv/rho_water`.

DEFINITIONS

Now, define the phase transition function as follows.

Interpolation 1 (int1)

- 1 In the **Home** toolbar, click  **Functions** and choose **Local>Interpolation**.

- 2 In the **Settings** window for **Interpolation**, locate the **Definition** section.
- 3 In the **Function name** text field, type `f_phtr`.
- 4 In the table, enter the following settings:

t	f(t)
-4	Sw_res
-1	Sw_res
0	1
6	1

- 5 Locate the **Units** section. In the **Function** table, enter the following settings:

Function	Unit
f_phtr	1

- 6 In the **Argument** table, enter the following settings:

Argument	Unit
t	degC

- 7 Click  **Plot**.

HEAT TRANSFER IN POROUS MEDIA (HT)

Add the soil properties next.

Porous Matrix I

- 1 In the **Model Builder** window, under **Component 1 (comp1)>Heat Transfer in Porous Media (ht)>Porous Medium 1** click **Porous Matrix 1**.
- 2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.
- 3 From the ϵ_p list, choose **User defined**. In the associated text field, type `por`.
- 4 From the **Define** list, choose **Solid phase properties**.
- 5 Locate the **Heat Conduction, Porous Matrix** section. From the k_s list, choose **User defined**. In the associated text field, type `k_solid`.
- 6 Locate the **Thermodynamics, Porous Matrix** section. From the ρ_s list, choose **User defined**. In the associated text field, type `rho_solid`.
- 7 From the $C_{p,s}$ list, choose **User defined**. In the associated text field, type `Cv/rho_solid`.

Initial Values 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)> Heat Transfer in Porous Media (ht)** click **Initial Values 1**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the T text field, type T_{init} .

Temperature 1

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Temperature**.
- 2 Select Boundary 1 only.
- 3 In the **Settings** window for **Temperature**, locate the **Temperature** section.
- 4 In the T_0 text field, type T_{in} .

MESH 1

As the model is cooled from one end of the domain, the mesh is created to resolve the area with the highest temperature gradient best.

Edge 1

In the **Mesh** toolbar, click  **Edge**.

Distribution 1

- 1 Right-click **Edge 1** and choose **Distribution**.
- 2 In the **Settings** window for **Distribution**, locate the **Distribution** section.
- 3 From the **Distribution type** list, choose **Predefined**.
- 4 In the **Number of elements** text field, type 100.
- 5 In the **Element ratio** text field, type 10.

Edge 1

In the **Model Builder** window, right-click **Edge 1** and choose **Build All**.

STUDY 1

Now set up the study with output times after 1, 2, and 3 days.

Step 1: Time Dependent

- 1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
- 3 From the **Time unit** list, choose **h**.
- 4 In the **Output times** text field, type 0 24 48 72.

The time step has to be small enough to catch the temperature decrease and the phase change correctly. Therefore, restrict the maximum time step to 2 minutes.

Solution I (solI)

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution I (solI)** node, then click **Time-Dependent Solver I**.
- 3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.
- 4 From the **Maximum step constraint** list, choose **Constant**.
- 5 In the **Maximum step** text field, type 2[**min**].
- 6 In the **Study** toolbar, click  **Compute**.

RESULTS

Temperature (ht)

Per default, the temperature is plotted. With the next steps you can change the temperature unit to degC and add a legend to the plot.

- 1 In the **Settings** window for **ID Plot Group**, locate the **Data** section.
- 2 From the **Time selection** list, choose **From list**.
- 3 In the **Times (h)** list, choose **24, 48, and 72**.
- 4 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.
- 5 From the **Position** list, choose **Bottom**.

Line Graph

- 1 In the **Model Builder** window, expand the **Temperature (ht)** node, then click **Line Graph**.
- 2 In the **Settings** window for **Line Graph**, locate the **y-Axis Data** section.
- 3 From the **Unit** list, choose **degC**.
- 4 Click to expand the **Legends** section. Select the **Show legends** check box.

Table I

The analytical solution provided by [Ref. 1](#) is available in a text file. Load it into the model and plot it to compare.

- 1 In the **Results** toolbar, click  **Table**.
- 2 In the **Settings** window for **Table**, locate the **Data** section.
- 3 Click **Import**.

- 4 Browse to the model's Application Libraries folder and double-click the file `phase_change_lunardini_analytical_solution.txt`.

Table Graph 1

- 1 In the **Model Builder** window, right-click **Temperature (ht)** and choose **Table Graph**.
- 2 In the **Settings** window for **Table Graph**, locate the **Coloring and Style** section.
- 3 Find the **Line style** subsection. From the **Line** list, choose **None**.
- 4 From the **Color** list, choose **Cycle (reset)**.
- 5 Find the **Line markers** subsection. From the **Marker** list, choose **Asterisk**.
- 6 From the **Positioning** list, choose **Interpolated**.
- 7 In the **Number** text field, type 25.

Temperature (ht)

- 1 In the **Model Builder** window, click **Temperature (ht)**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Axis** section.
- 3 Select the **Manual axis limits** check box.
- 4 In the **x maximum** text field, type 5.
- 5 In the **Temperature (ht)** toolbar, click  **Plot**. Compare with [Figure 1](#)

