Phase Change

Introduction

This example demonstrates how to model a phase change and predict its impact on a heat transfer analysis. When a material changes phase, for instance from solid to liquid, energy is added to the solid. Instead of creating a temperature rise, the energy alters the material's molecular structure. Heat consumed or released by a phase change affects fluid flow, magma movement and production, chemical reactions, mineral stability, and many other earth-science applications.

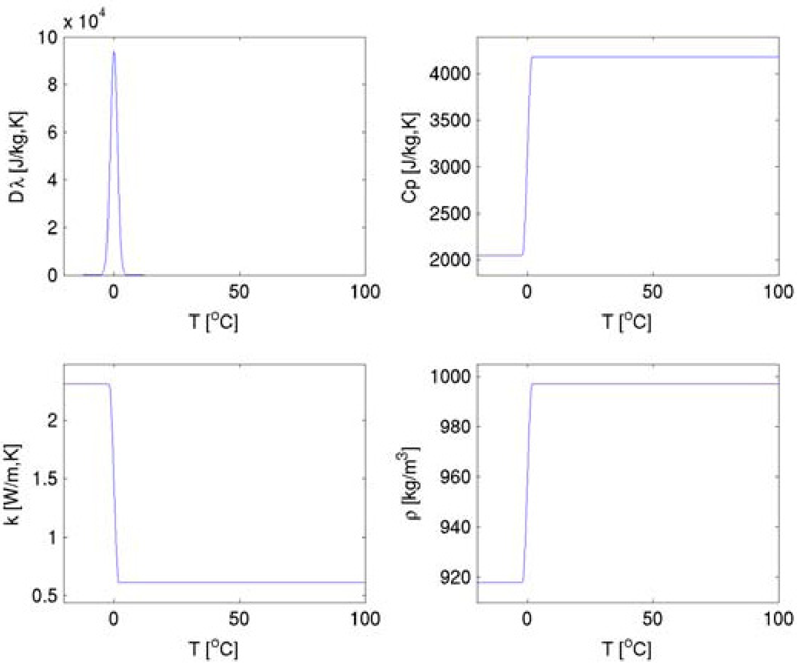


Figure 1: Material properties as functions of temperature.

This 1D example uses the Heat Transfer with Phase Change feature from the Heat Transfer Module to examine transient temperature transfer in a rod of ice that heats up and changes to water. In particular, the model demonstrates how to handle material properties that vary as a function of temperature.

This model proceeds as follows. First, estimate the ice-to-water phase change using the transient conduction equation with the latent heat of fusion. Next, compare the first solution to estimates that neglect latent heat. Finally, run additional simulations to evaluate impacts of the temperature interval over which the phase change occurs.

Model Definition

This example describes the ice-to-water phase change along a 1-cm rod of ice. At its left end the rod is insulated, and at the other temperature is maintained at 80 °C. Values for thermal properties depend on the phase. They are presented in Table 1, at 265 K for ice and 300 K for water.

TABLE 1: MATERIAL PROPERTIES OF ICE AND WATER

MATERIAL PROPERTY	ICE (AT 265 K)	WATER (AT 300 K)
Density	918 kg/m^3	997 kg/m^3
Heat capacity at constant pressure	2052 J/(kg·K)	4179 J(kg·K)
Thermal conductivity	2.31 W/(m·K)	0.613 W/(m·K)

The latent heat of fusion, l_m, is 333.5 kJ/kg and the rod is initially at –20 °C.

During the ice-to-water phase change, the density is modified, resulting in a volume compression. The material coordinates express all transformations in the initial coordinate system, when ice occupies all the domain. Assuming that there is no mixing in the liquid phase, the conduction equation in material coordinates can be used. It simplifies the model since you do not need to calculate the velocity field resulting from density variations during phase change. The conduction equation in material coordinates reads

$$\rho C_{eq}\frac{\partial T}{\partial t} + \nabla \cdot (-k_{eq}\nabla T) = Q \tag{1}$$

where ρ (kg/m^3) is the density, C_{eq} (J/kg·K) is the effective heat capacity at constant pressure, k_{eq} is the effective thermal conductivity (W/m·K), T is temperature (K), and Q is a heat source (W/m^3).

The material properties ρ and k_{eq} of water must be in material coordinates. Because values given in Table 1 come from measurements, they correspond to spatial coordinates. Hence, conversion into material coordinates is necessary. In 1D models, you just have to multiply by the ratio of densities, ρ_{ratio}:

$$\rho_{\mathrm{ratio}} = \frac{\rho_{\mathrm{ice}}}{\rho_{\mathrm{water}}}$$

Note: With this transformation, the density of water, ρ, in material coordinates is $\rho = \rho_{\mathrm{water}}\rho_{\mathrm{ratio}} = \rho_{\mathrm{ice}}$. This is consistent with conservation of mass because the integral of ρ over the geometry domain remains constant in time.

The boundary conditions for this model are

- thermal insulation at $x = 0$;
- fixed temperature at $x = 0.01$; the fixed temperature creates a temperature discontinuity at the starting time. You can thus replace T_{hot} by a smoothed step function T_{right} that increases the temperature from T_0 to T_{hot} in 0.1 s.

Results and Discussion

Figure 2 shows images of the temperature distribution in time, predicted with latent heat. The system is solid ice at $t = 0$, and water content increases with time.

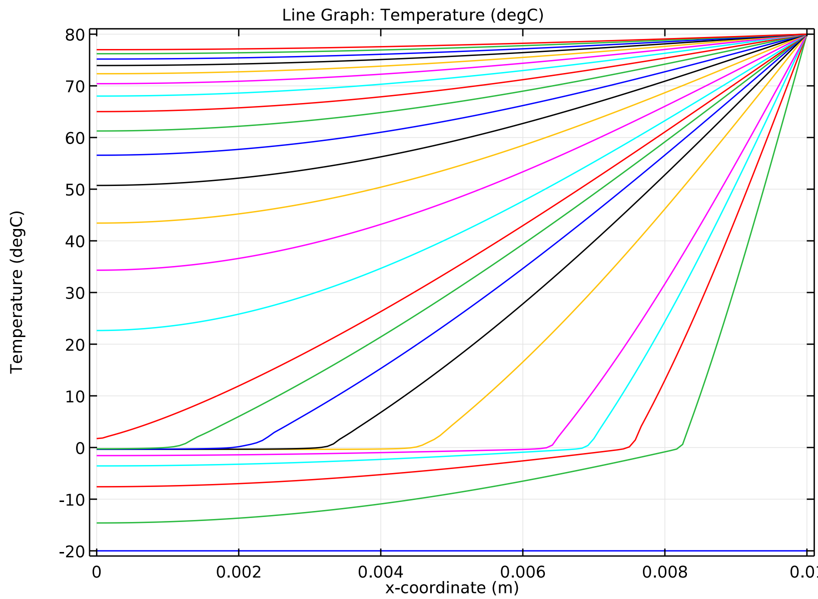


Figure 2: Temperature estimates with latent heat at t = 0 s, 15 s, 30 s, 45 s, 60 s, 2 min, 3 min, 4 min, …, 20 min.

The distributions all level out around the 0 °C temperature point because not all of the energy is going toward a temperature rise; some is being absorbed to change the molecular structure and change the phase.

The solution in Figure 3 shows temperature estimates for the simulation without latent heat.

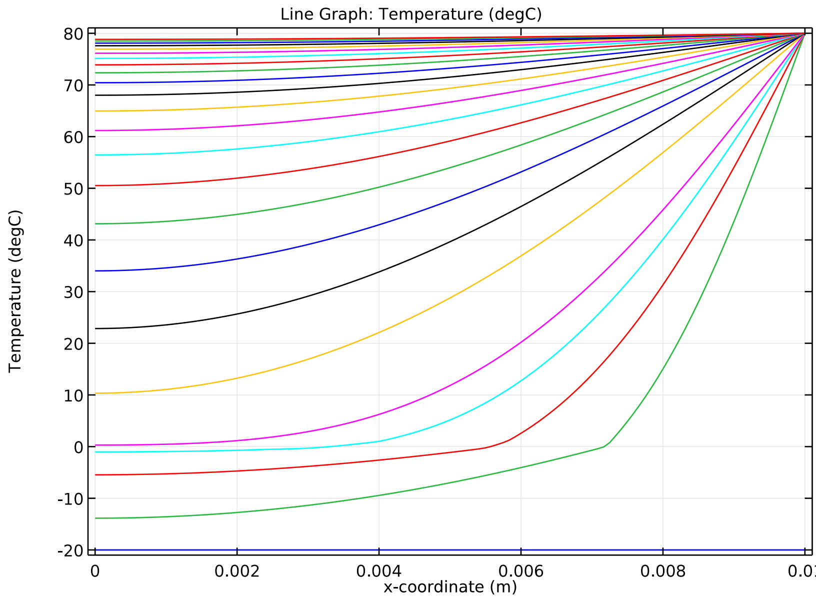


Figure 3: Temperature estimates without latent heat at t = 0 s, 15 s, 30 s, 45 s, 60 s, 2 min, 3 min, 4 min, …, 20 min.

A change of profile also occurs at 0 °C but is less visible. Because latent heat is not accounted for, this change is here due to the different thermophysical properties of water below and above 0 °C.

Figure 4 shows results for different solid-to-liquid intervals at three times. The smaller the interval, the sharper the bend in the temperature profile at zero temperature, T. In the simulations, narrowing the temperature interval to a step change, for example, comes at a large computational cost. In the figure, the results for the wide and narrow pulses compare closely.

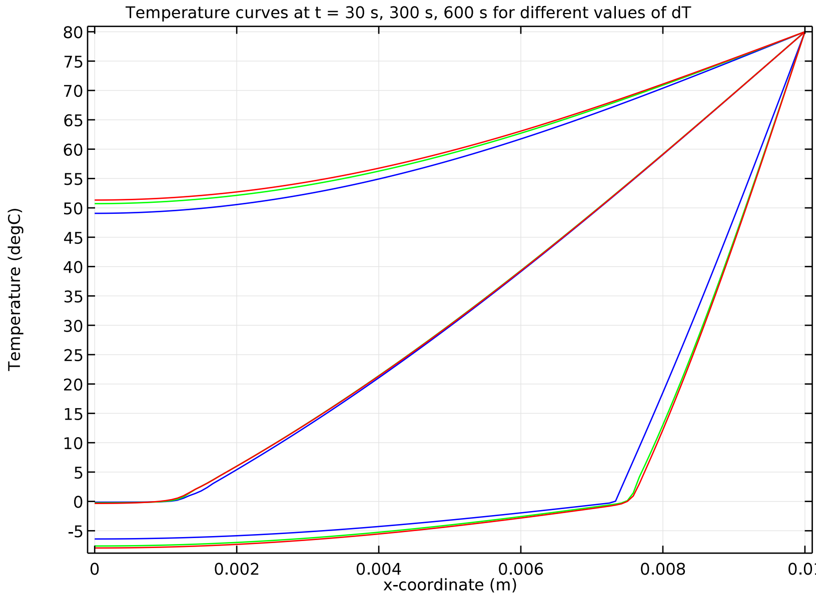


Figure 4: Temperature estimates for different temperature intervals for latent heat consumption. Estimates are for dT intervals of 0.5 K (blue), 1 K (green), and 2 K (red) at t = 30 s (three curves at bottom), 5 min (three curves at middle), and 10 min (three curves on top).

References

1. S.E. Ingebritsen and W.E. Sanford, *Groundwater in Geologic Processes*, Cambridge University Press, 1998.

2. N.H. Sleep and K. Fujita, *Principles of Geophysics*, Blackwell Science, 1997.

3. D.L. Turcotte and G. Schubert, *Geodynamics: Applications of Continuum Physics to Geological Problems*, 2nd ed., Cambridge University Press, 2002.

Application Library path: `Subsurface_Flow_Module/Heat_Transfer/phase_change`

Modeling Instructions

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

NEW

1 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>Heat Transfer in Fluids (ht)**.

The **Heat Transfer in Fluids** interface with its **Heat Transfer with Phase Change** feature solves for the temperature and automatically calculates the equivalent conductivity and the equivalent specific heat capacity.

3 Click **Add**.

4 Click **Study**.

5 In the **Select study** tree, select **Preset Studies>Time Dependent**.

6 Click **Done**.

GEOMETRY 1

Interval 1 (i1)

1 On the **Geometry** toolbar, click **Interval**.

2 In the **Settings** window for Interval, locate the **Interval** section.

3 In the **Right endpoint** text field, type `0.01`.

Form Union (fin)

1 Right-click **Interval 1 (i1)** and choose **Build Selected**.

2 In the **Model Builder** window, under **Component 1 (comp1)>Geometry 1** right-click **Form Union (fin)** and choose **Build Selected**.

3 Click the **Zoom Extents** button on the **Graphics** toolbar.

GLOBAL DEFINITIONS

The following steps describe how the model parameters are defined.

Parameters

1 On the **Home** toolbar, click **Parameters**.

2 In the **Settings** window for Parameters, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
T_trans	0[degC]	273.2 K	Transition temperature
dT	1[K]	1 K	Transition interval
lm	333.5[kJ/kg]	3.335E5 J/kg	Latent heat of fusion
T_0	-20[degC]	253.1 K	Initial temperature of the rod
T_hot	80[degC]	353.2 K	Temperature of hot water
rho_ice	918[kg/m^3]	918 kg/m³	Density of ice
rho_water	997[kg/m^3]	997 kg/m³	Density of water
rho_ratio	rho_ice/ rho_water	0.9208	Ratio of densities

Step 1 (step1)

1 On the **Home** toolbar, click **Functions** and choose **Global>Step**.

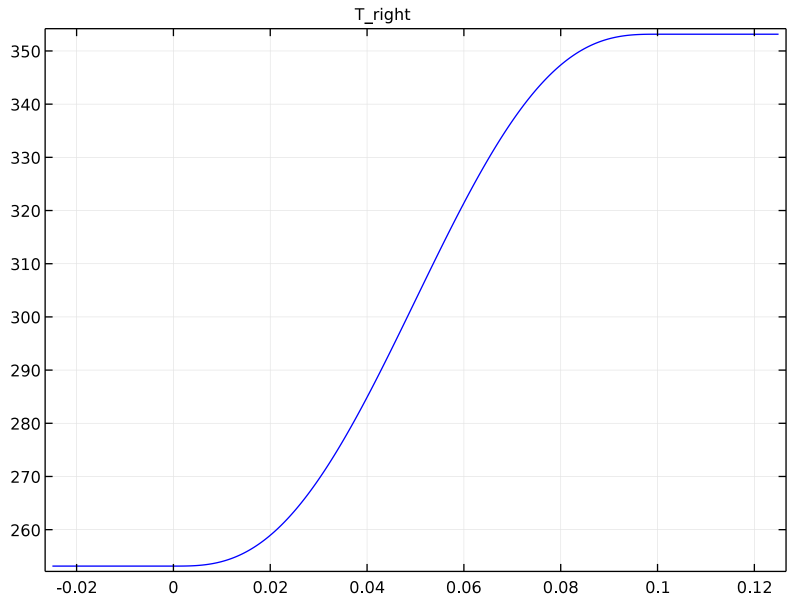
2 In the **Settings** window for Step, type `T_right` in the **Function name** text field.

3 Locate the **Parameters** section. In the **Location** text field, type `0.05`.

4 In the **From** text field, type `T_0`.

5 In the **To** text field, type `T_hot`.

6 Click to expand the **Smoothing** section. Click the **Plot** button.



MATERIALS

Material 1 (mat1)

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for Material, type `Ice` in the **Label** text field.

3 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Thermal conductivity	k	2.31	W/(m·K)	Basic
Density	rho	rho_ice	kg/m³	Basic
Heat capacity at constant pressure	Cp	2052	J/(kg·K)	Basic
Ratio of specific heats	gamma	1	1	Basic

Material 2 (mat2)

1 Right-click **Materials** and choose **Blank Material**.

2 In the **Settings** window for Material, type `Water` in the **Label** text field.

3 Select Domain 1 only.

Because the model is solved in material coordinates, the water density and thermal conductivity are converted.

4 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Name	Value	Unit	Property group
Thermal conductivity	k	`0.613[W/(m*K)]*rho_ratio`	W/(m·K)	Basic
Density	rho	`rho_water*rho_ratio`	kg/m³	Basic
Heat capacity at constant pressure	Cp	`4179`	J/(kg·K)	Basic
Ratio of specific heats	gamma	`1`	1	Basic

HEAT TRANSFER IN FLUIDS (HT)

Heat Transfer with Phase Change 1

1 On the **Physics** toolbar, click **Domains** and choose **Heat Transfer with Phase Change**.

2 Select Domain 1 only.

3 In the **Settings** window for Heat Transfer with Phase Change, locate the **Phase Change** section.

4 In the $\Delta T_{1\mathrm{to}2}$ text field, type `dT`.

5 In the $L_{1\mathrm{to}2}$ text field, type `lm`.

6 Locate the **Phase 1** section. From the **Material, phase 1** list, choose **Ice (mat1)**.

7 Locate the **Phase 2** section. From the **Material, phase 2** list, choose **Water (mat2)**.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Heat Transfer in Fluids (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_0`.

Temperature 1

1 On the **Physics** toolbar, click **Boundaries** and choose **Temperature**.

2 Select Boundary 2 only.

3 In the **Settings** window for Temperature, locate the **Temperature** section.

4 In the T_0 text field, type T_right(t[1/s]).

MESH 1

Follow the steps below to generate a relatively fine mesh of 120 elements.

Edge 1

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Edge**.

Distribution 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** right-click **Edge 1** and choose **Distribution**.

2 In the **Settings** window for Distribution, locate the **Distribution** section.

3 In the **Number of elements** text field, type 120.

4 Click the **Build Selected** button.

STUDY 1

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 Click **Range**.

4 In the **Range** dialog box, type 15 in the **Step** text field.

5 In the **Stop** text field, type 60.

6 Click **Replace**.

7 In the **Settings** window for Time Dependent, locate the **Study Settings** section.

8 Click **Range**.

9 In the **Range** dialog box, type 120 in the **Start** text field.

10 In the **Step** text field, type 60.

11 In the **Stop** text field, type 1200.

12 Click **Add**.

13 In the **Settings** window for Time Dependent, locate the **Study Settings** section.

14 Select the **Relative tolerance** check box.

15 In the associated text field, type 0.001.

16 On the **Home** toolbar, click **Compute**.

RESULTS

Temperature (ht)

All the parameter values in this model have a time unit of seconds, so the output time you enter here gives a total simulation time of 20 minutes. Different output intervals can be generated by adding other range commands as it is done above. Within the first minute, solution data is stored every 15 seconds, whereas for the remaining simulation period, the data is only stored every 60 seconds.

A line plot of the temperature distribution along the rod for all times is automatically produced. To generate Figure 2, you only need to change the temperature unit.

1 In the **Model Builder** window, expand the **Temperature (ht)** node, then click **Line Graph 1**.
2 In the **Settings** window for Line Graph, locate the **y-Axis Data** section.
3 From the **Unit** list, choose **degC**.
4 On the **Temperature (ht)** toolbar, click **Plot**.

Phase Change Without Latent Heat

To analyze the impact of the latent heat terms on the phase change model, it is useful to estimate temperatures using the same approach but without the latent heat term. Therefore, latent heat `lm` is just set to zero. To keep the original value of 333.5 kJ/kg, introduce the parameter `lm_original`.

GLOBAL DEFINITIONS

Parameters

1 In the **Model Builder** window, under **Global Definitions** click **Parameters**.
2 In the **Settings** window for Parameters, locate the **Parameters** section.
3 In the table, enter the following settings:

Name	Expression	Value	Description
lm	0	0	Latent heat of fusion
lm_original	333.5[kJ/kg]	3.335E5 J/kg	Latent heat of fusion, original

ADD STUDY

1 On the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select study** tree, select **Preset Studies**.

4 In the **Select study** tree, select **Preset Studies>Time Dependent**.

5 Click **Add Study** in the window toolbar.

STUDY 2

Step 1: Time Dependent

1 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

2 In the **Model Builder** window, under **Study 2** click **Step 1: Time Dependent**.

3 In the **Settings** window for Time Dependent, locate the **Study Settings** section.

4 Click **Range**.

5 In the **Range** dialog box, type `60` in the **Stop** text field.

6 In the **Step** text field, type `15`.

7 Click **Replace**.

8 In the **Settings** window for Time Dependent, locate the **Study Settings** section.

9 Click **Range**.

10 In the **Range** dialog box, type `120` in the **Start** text field.

11 In the **Stop** text field, type `1200`.

12 In the **Step** text field, type `60`.

13 Click **Add**.

14 In the **Settings** window for Time Dependent, locate the **Study Settings** section.

15 Select the **Relative tolerance** check box.

16 In the associated text field, type `0.001`.

17 On the **Home** toolbar, click **Compute**.

RESULTS

Temperature (ht) 1

1 In the **Settings** window for 1D Plot Group, type `Temperature, No Latent Heat` in the **Label** text field.

To generate Figure 3, you only need to change the units in the automatically generated temperature plot.

Temperature, No Latent Heat

1 In the **Model Builder** window, expand the **Results>Temperature, No Latent Heat** node, then click **Line Graph 1**.

2 In the **Settings** window for Line Graph, locate the **y-Axis Data** section.

3 From the **Unit** list, choose **degC**.

4 On the **Temperature, No Latent Heat** toolbar, click **Plot**.

To be able to keep track of the different studies, rename the data sets containing the solutions of **Study 1** and **Study 2**.

Data Sets

1 In the **Model Builder** window, expand the **Results>Data Sets** node, then click **Study 1/Solution 1 (sol1)**.

2 In the **Settings** window for Solution, type `Solution 1, lm Included` in the **Label** text field.

3 In the **Model Builder** window, under **Results>Data Sets** click **Study 2/Solution 2 (sol2)**.

4 In the **Settings** window for Solution, type `Solution 2, lm Excluded` in the **Label** text field.

Phase Change for Varying Transition Intervals

Solutions to the phase change problem vary with the range in temperatures `dT` over which you assume that the phase transition occurs. To visualize the impact of different transition widths sample results from the original simulation and compare those estimates to results from simulations with varying `dT` values.

GLOBAL DEFINITIONS

Parameters

1 In the **Model Builder** window, under **Global Definitions** click **Parameters**.

2 In the **Settings** window for Parameters, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	**Expression**	**Value**	**Description**
`lm`	`lm_original`	3.335E5 J/kg	`Latent heat of fusion`

ADD STUDY

1 On the **Home** toolbar, click **Add Study** to open the **Add Study** window.

2 Go to the **Add Study** window.

3 Find the **Studies** subsection. In the **Select study** tree, select **Preset Studies**.

4 In the **Select study** tree, select **Preset Studies>Time Dependent**.

5 Click **Add Study** in the window toolbar.

STUDY 3

Step 1: Time Dependent

1 On the **Home** toolbar, click **Add Study** to close the **Add Study** window.

2 In the **Model Builder** window, under **Study 3** click **Step 1: Time Dependent**.

3 In the **Settings** window for Time Dependent, locate the **Study Settings** section.

4 Click **Range**.

5 In the **Range** dialog box, type `60` in the **Stop** text field.

6 In the **Step** text field, type `15`.

7 Click **Replace**.

8 In the **Settings** window for Time Dependent, locate the **Study Settings** section.

9 Click **Range**.

10 In the **Range** dialog box, type `120` in the **Start** text field.

11 In the **Stop** text field, type `1200`.

12 In the **Step** text field, type `60`.

13 Click **Add**.

14 In the **Settings** window for Time Dependent, locate the **Study Settings** section.

15 Select the **Relative tolerance** check box.

16 In the associated text field, type `0.001`.

Follow the steps below to calculate the temperature distribution of the rod for different values of the transition interval by just adding a parametric sweep to the study node. In this example, use the values 0.1 K, 0.5 K, and 2.5 K for `dT`.

Parametric Sweep

1 On the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for Parametric Sweep, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
dT	0.5 1 2	

5 On the **Study** toolbar, click **Compute**.

RESULTS

Temperature (ht) 1

Again, the temperature distribution along the rod for all time steps and `dT`-values is produced automatically. You can modify this plot to generate Figure 4 by following the steps below.

1 In the **Settings** window for 1D Plot Group, click to expand the **Title** section.

2 From the **Title type** list, choose **Manual**.

3 In the **Title** text area, type `Temperature curves at t = 30 s, 300 s, 600 s for different values of dT`.

4 In the **Model Builder** window, expand the **Temperature (ht) 1** node, then click **Line Graph 1**.

5 In the **Settings** window for Line Graph, locate the **Data** section.

6 From the **Data set** list, choose **Study 3/Parametric Solutions 1 (sol4)**.

7 From the **Parameter selection (dT)** list, choose **First**.

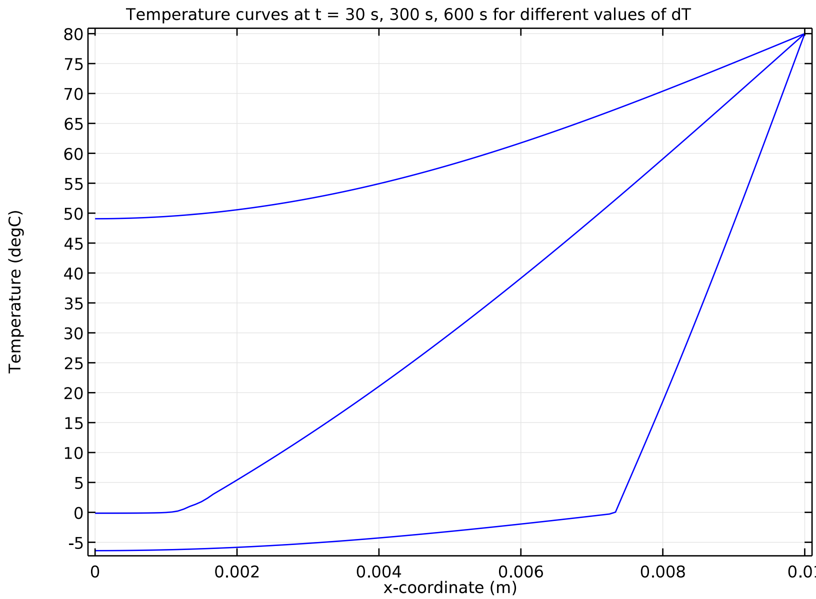
8 From the **Time selection** list, choose **Interpolated**.

9 In the **Times (s)** text field, type `30 300 600`.

10 Locate the **y-Axis Data** section. From the **Unit** list, choose **degC**.

11 Click to expand the **Coloring and style** section. Locate the **Coloring and Style** section. From the **Color** list, choose **Blue**.

12 On the **Temperature (ht) 1** toolbar, click **Plot**.



13 Right-click **Results>Temperature (ht) 1>Line Graph 1** and choose **Duplicate**.

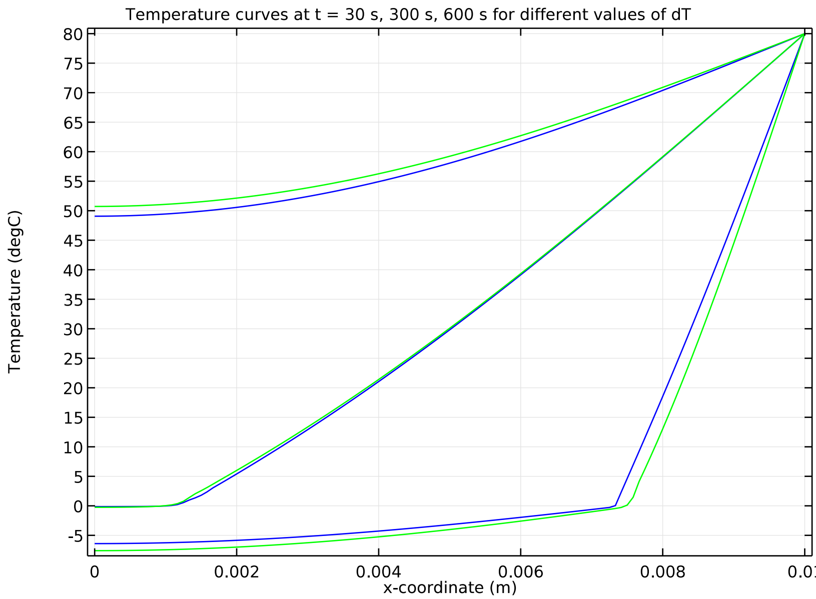
14 In the **Settings** window for Line Graph, locate the **Data** section.

15 From the **Parameter selection (dT)** list, choose **From list**.

16 In the **Parameter values (dT)** list, select **1**.

17 Locate the **Coloring and Style** section. From the **Color** list, choose **Green**.

18 On the **Temperature (ht) 1** toolbar, click **Plot**.



19 Right-click **Line Graph 1** and choose **Duplicate**.

20 In the **Settings** window for Line Graph, locate the **Data** section.

21 From the **Parameter selection (dT)** list, choose **Last**.

22 Locate the **Coloring and Style** section. From the **Color** list, choose **Red**.

23 On the **Temperature (ht) 1** toolbar, click **Plot**.

24 In the **Model Builder** window, click **Temperature (ht) 1**.

25 In the **Settings** window for 1D Plot Group, type `Temperature, Varying dT` in the **Label** text field.