Model created in COMSOL Multiphysics 6.4

Phase Change

Introduction

This example demonstrates how to model a phase change and predicts 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.

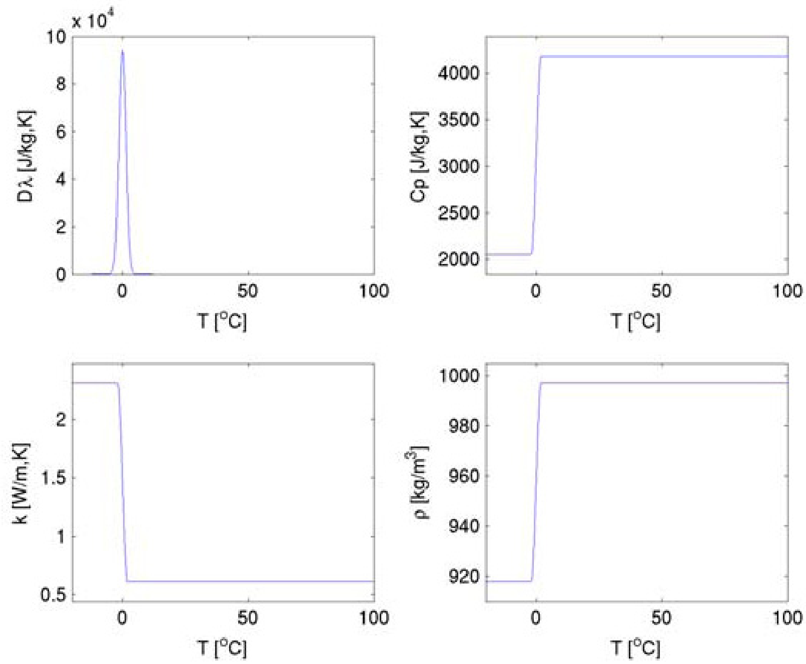


Figure 1: Material properties as functions of temperature.

This 1D example uses the Phase Change Material subfeature 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 –8°C for ice and 27°C for water.

TABLE 1: MATERIAL PROPERTIES OF ICE AND WATER

MATERIAL PROPERTY	ICE (AT -8°C)	WATER (AT 27°C)
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}:

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

Note: With this transformation, the density of water, ρ, in material coordinates is $\rho = \rho_{water}\rho_{ratio} = \rho_{ice}$. 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 $x = 0$ m;
- fixed temperature at $x = 0.01$ m; the fixed temperature creates a temperature discontinuity at the start 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 the spatial distribution of temperature at different times, from t = 0 s to t = 20 min, predicted with latent heat. The system is solid ice at $t = 0$ s, and water content increases with time.

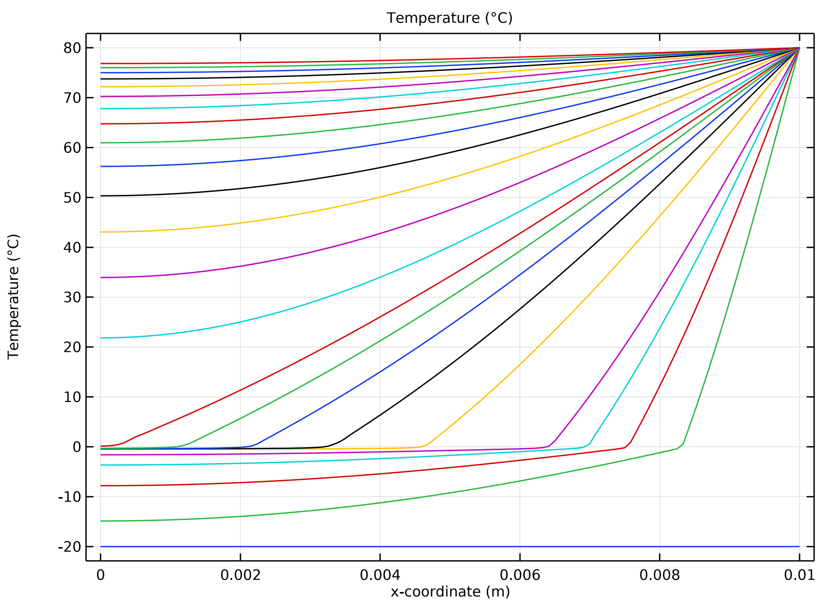


Figure 2: Temperature estimates with latent heat at t = 0 s, 15 s, 30 s, 45 s, 60 s, 2 min, 3 min, 4 min, …, 20 min.

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.

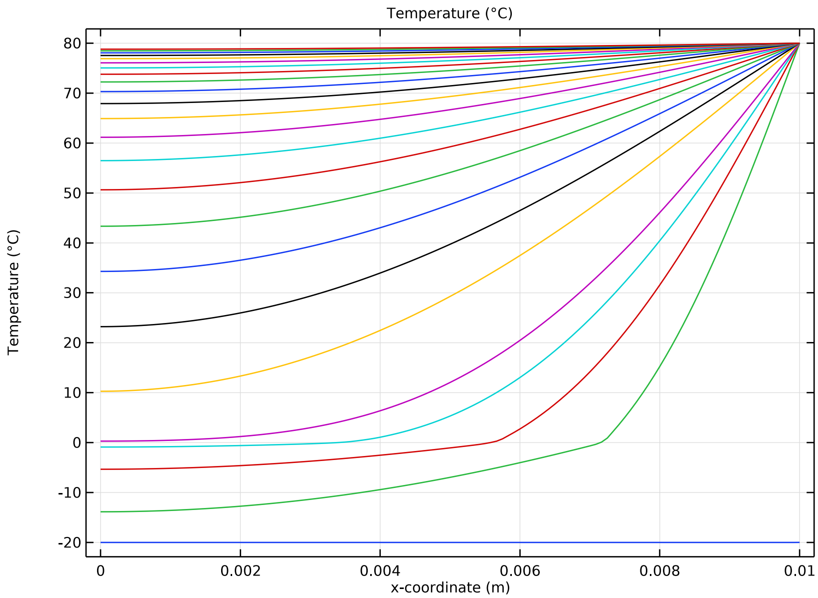


Figure 3: Temperature estimates without latent heat at t = 0 s, 15 s, 30 s, 45 s, 60 s, 2 min, 3 min, 4 min, …, 20 min.

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.

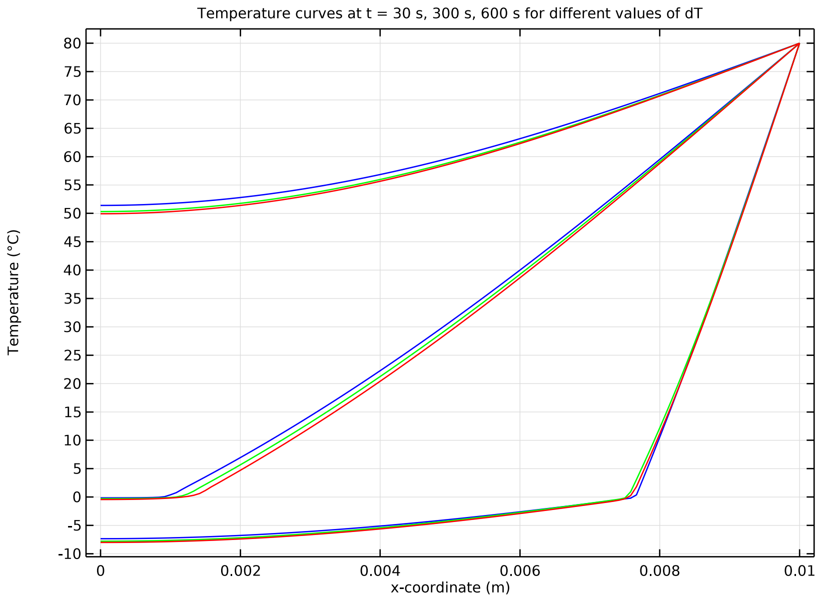


Figure 4: Temperature estimates for different temperature intervals for latent heat consumption. Estimates are for dT intervals of 0.5°C (blue), 1°C (green), and 2°C (red) at t = 30 s (three curves at bottom), 5 min (three curves at middle), and 10 min (three curves on top).

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: `Heat_Transfer_Module/Phase_Change/phase_change`

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

The **Heat Transfer in Fluids** interface with its **Fluid** feature together with the **Phase Change Material** subfeature 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 **General Studies** > **Time Dependent**.

6 Click **Done**.

GEOMETRY 1

Interval 1 (i1)

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
0.01

4 Click **Build Selected**.

Form Union (fin)

1 In the **Model Builder** window, click **Form Union (fin)**.

2 In the **Settings** window for **Form Union/Assembly**, click **Build Selected**.

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

GLOBAL DEFINITIONS

The following steps describe how the model parameters are defined.

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 In the table, enter the following settings:

Name	Expression	Value	Description
T_trans	0[degC]	273.15 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]	253.15 K	Initial temperature of the rod
T_hot	80[degC]	353.15 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	0.92076	Ratio of densities

Step 1 (step1)

1 In the **Home** toolbar, click f(X) **Functions** and choose **Global** > **Step**.

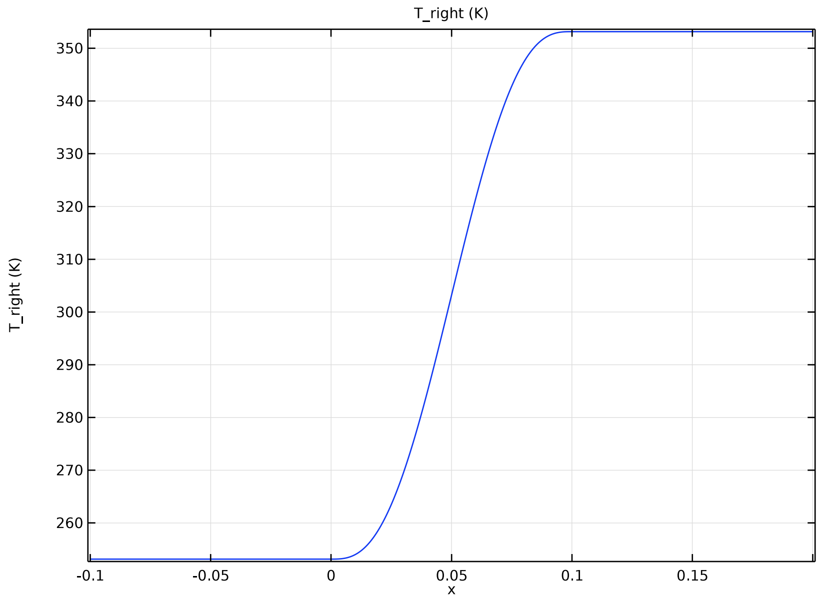
2 In the **Settings** window for **Step**, type T_right in the **Function name** text field.

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 **Plot**.



MATERIALS

Ice

1 In the **Materials** toolbar, click **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	Variable	Value	Unit	Property group
Heat capacity at constant pressure	Cp	`2052[J/(kg*K)]`	J/(kg·K)	Basic
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	`2.31[W/(m*K)]`	W/(m·K)	Basic
Density	rho	`rho_ice`	kg/m³	Basic

Water

1 In the **Materials** toolbar, click **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	Variable	Value	Unit	Property group
Heat capacity at constant pressure	Cp	`4179[J/(kg*K)]`	J/(kg·K)	Basic
Thermal conductivity	k_iso ; kii = k_iso, kij = 0	`0.613[W/(m*K)]*rho_ratio`	W/(m·K)	Basic
Density	rho	`rho_water*rho_ratio`	kg/m³	Basic

HEAT TRANSFER IN FLUIDS (HT)

Fluid 1

In the **Model Builder** window, under **Component 1 (comp1)** > **Heat Transfer in Fluids (ht)** 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 In the $\Delta T_{1 \to 2}$ text field, type `dT`.

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

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

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

4 Click **Build Selected**.

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, 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, 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**.

For more robust convergence, tighten the relative tolerance, which controls the size of the time steps taken by the solver.

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

14 From the **Tolerance** list, choose **User controlled**.

15 In the **Relative tolerance** text field, type `1e-3`.

16 In the **Study** toolbar, click **Compute**.

RESULTS

Change the unit of the temperature results to degrees Celsius.

Preferred Units 1

1. In the **Results** toolbar, click **Configurations** and choose **Preferred Units**.
2. In the **Settings** window for **Preferred Units**, locate the **Units** section.
3. Click **Add Physical Quantity**.
4. In the **Physical Quantity** dialog, select **General** > **Temperature (K)** in the tree.
5. Click **OK**.
6. In the **Settings** window for **Preferred Units**, locate the **Units** section.
7. In the table, enter the following settings:

Quantity	Unit	Preferred unit
Temperature	K	°C

8. Click **Apply**.

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.

Line Graph 1

1. In the **Model Builder** window, expand the **Temperature (ht)** node, then click **Line Graph 1**.
2. In 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, a parametric sweep with a single value is used to set the latent heat to 0 in a new study.

ADD STUDY

1 In 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 **General Studies** > **Time Dependent**.

4 Click the **Add Study** button in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 2

Step 1: Time Dependent

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

2 Click **Range**.

3 In the **Range** dialog, type 60 in the **Stop** text field.

4 In the **Step** text field, type 15.

5 Click **Replace**.

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

7 Click **Range**.

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

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

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

11 Click **Add**.

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

13 From the **Tolerance** list, choose **User controlled**.

14 In the **Relative tolerance** text field, type 1e-3.

15 Click to expand the **Study Extensions** section. Select the **Auxiliary sweep** checkbox.

16 Click **Add**.

17 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
lm (Latent heat of fusion)	0	J/kg

18 In the **Study** toolbar, click **Compute**.

RESULTS

Temperature, No Latent Heat

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.

Line Graph 1

1. In the **Model Builder** window, expand the **Temperature, No Latent Heat** node, then click **Line Graph 1**.
2. In the **Temperature, No Latent Heat** toolbar, click **Plot**.

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

Solution 1, lm Included

1. In the **Model Builder** window, expand the **Results** > **Datasets** 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.

Solution 2, lm Excluded

1. In the **Model Builder** window, under **Results** > **Datasets** click **Study 2/Solution 2 (sol2)**.
2. 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.

ADD STUDY

1. In 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 **General Studies** > **Time Dependent**.

4 Click the **Add Study** button in the window toolbar.

5 In the **Home** toolbar, click **Add Study** to close the **Add Study** window.

STUDY 3

Step 1: Time Dependent

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

2 Click **Range**.

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

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

5 Click **Replace**.

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

7 Click **Range**.

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

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

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

11 Click **Add**.

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

13 From the **Tolerance** list, choose **User controlled**.

14 In the **Relative tolerance** text field, type `1e-3`.

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 0.5 K, 1 K, and 2 K for `dT`.

Parametric Sweep

1 In 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 (Transition interval)	0.5 1 2	K

5 In 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`.

Line Graph 1

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

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

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

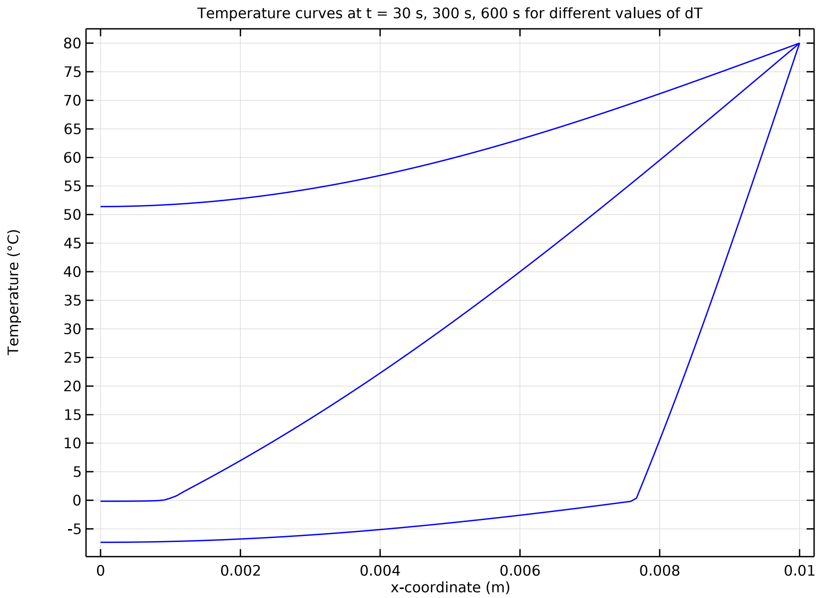
4 From the **Parameter selection (dT)** list, choose **First**.

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

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

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

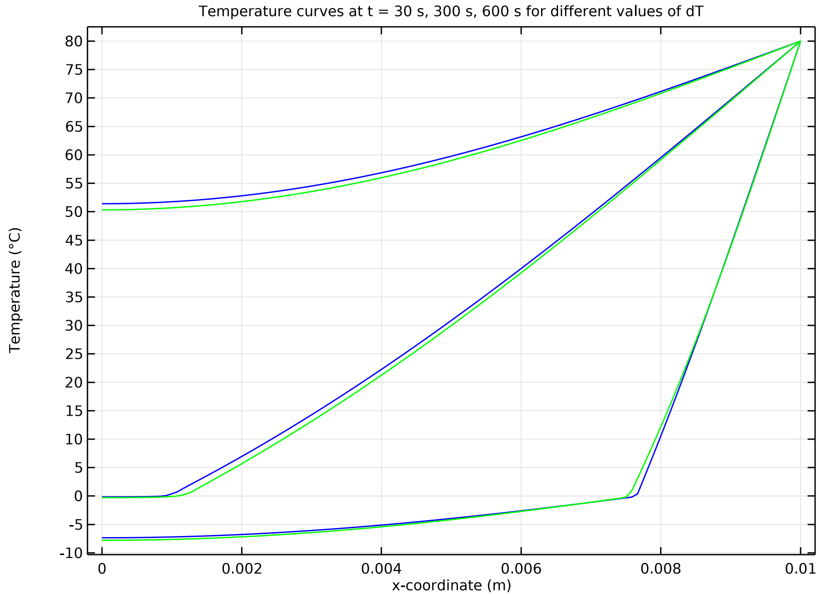
8 In the **Temperature (ht) 1** toolbar, click **Plot**.



Line Graph 2

1. Right-click **Results** > **Temperature (ht) 1** > **Line Graph 1** and choose **Duplicate**.
2. In the **Settings** window for **Line Graph**, locate the **Data** section.
3. From the **Parameter selection (dT)** list, choose **From list**.
4. In the **Parameter values (dT (K))** list box, select **1**.
5. Locate the **Coloring and Style** section. From the **Color** list, choose **Green**.

6 In the **Temperature (ht) 1** toolbar, click **Plot**.



Line Graph 3

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

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

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

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

5 In the **Temperature (ht) 1** toolbar, click **Plot**.

Temperature, Varying dT

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

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