Spherically Symmetric Transport

Introduction

Many models of industrial-transport problems allow the assumption that the problem is spherically symmetric. This assumption is of great importance because it eliminates two space coordinates and leaves a 1D problem that is computationally fast and has very small memory requirements. Some applications where spherical symmetry assumptions are useful include:

- Reaction and diffusion in catalytic pellets in chemical reactors
- Heat and mass transfer in the processing of upgraded iron-ore pellets
- Any other process that takes place in beads that are nearly spherical

For spherical symmetry to be valid, the following assumptions must apply:

- The computational domain has a spherical shape
- The outer-perimeter boundary condition does not change with the position on the surface, that is, it does not vary with the space angles θ and φ
- At any given time for a time-dependent problem, the material properties depend only on the radial distance from the center, r, and not on the space angles θ and φ
- For a time-dependent problem, the initial condition depends only on the radial distance from the center, r, and not on the space angles θ and φ

Model Definition

The following example simulates the initial transient heating process of a pelletized piece of magnetite ore. This is the first step in the process of making hematite ore pellets, an important raw material for the steel industry.

During the initial heating of a magnetite pellet the temperature is in a range that allows you to disregard any phase change of moisture. Thus it is possible to use a transient heat-conduction equation with constant properties in spherical symmetry. You can also scale the equation for easy parameterization of the radius.

Figure 1 depicts some pellets together with a push pin as a scale reference.

Figure 1: Hematite pellets after drying and oxidation (end product).

The figure shows that these pellets are indeed not perfectly spherical. Nonetheless, this model takes advantage of the assumption of spherical symmetry.

DOMAIN EQUATIONS

Starting with the time-dependent heat conduction equation

$$\rho c_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = Q$$

and expanding it in spherical polar coordinates, the result is the equation

$$\rho c_p \frac{\partial T}{\partial t} - k\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial T}{\partial r}\right) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial T}{\partial \theta}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2 T}{\partial \varphi^2}\right] = Q$$

where ρ is the density (kg/m^3), c_p gives the heat capacity (J/(kg·K)), k denotes the thermal conductivity (W/(m·K)), and Q is an internal heat source (W/m^3). Further, r, θ, and φ are the spatial coordinates.

Assuming a perfect sphere of radius R_p and no change in temperature with differing space angles, or $\partial T / \partial \theta = \partial T / \partial \varphi = 0$, gives

$$\rho c_p \frac{\partial T}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\left(-k r^2 \frac{\partial T}{\partial r}\right) = Q$$

To avoid division by zero at $r = 0$, which causes numerical problems, multiply this equation by r^2

$$r^2 \rho c_p \frac{\partial T}{\partial t} + \frac{\partial}{\partial r}\left(-k r^2 \frac{\partial T}{\partial r}\right) = r^2 Q \tag{1}$$

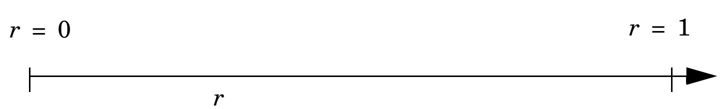
Using a dimensionless radial coordinate $\hat{r}$ by scaling the equation provides the option to quickly change the pellet's radius without changing or parameterizing the geometry size[1]. Introducing the dimensionless coordinate

$$\hat{r} = \frac{r}{R_p}, \quad \frac{\partial}{\partial r} = \frac{1}{R_p}\frac{\partial}{\partial \hat{r}}$$

and substituting in Equation 1 leads to

$$\hat{r}^2 \rho c_p \frac{\partial T}{\partial t} + \frac{\partial}{\partial \hat{r}}\left(\frac{-k\hat{r}^2}{R_p^2}\frac{\partial T}{\partial \hat{r}}\right) = \hat{r}^2 Q \tag{2}$$

on the following domain:



In a similar manner, it is possible to derive equations similar to Equation 2 for porous media flow, diffusion-reaction problems, and so on.

The model uses the following material data:

SYMBOL	NAME	VALUE
ρ	Density	2000 kg/m^3
c_p	Heat capacity	300 J/(kg·K)
k	Conductivity	0.5 W/(m·K)
R_p	Pellet radius	0.005 m
Q	Heat source	0 W/m^3

1. Note that scaling the variables to get well-conditioned problems is not necessary in COMSOL Multiphysics because the solvers use automatic variable scaling.

BOUNDARY CONDITIONS AND INITIAL CONDITIONS

Because of symmetry about $r = 0$, there is zero flux through this point, meaning $\partial T/\partial\hat{r} = 0$.

At the surface, $\hat{r} = 1$, you use a convective heating expression with a heat transfer coefficient, h_s (W/(m^2·K)), for the influx of heat (W/m^2):

$$q_{\text{in}} = h_s(T_{\text{ext}} - T)$$

This expression describes a hot gas with a temperature T_{ext} flowing around the pellet. T_{ext} is chosen at 95°C. The heat transfer coefficient is set to 1000 W/(m^2·K). The initial condition is set to 25°C.

Results

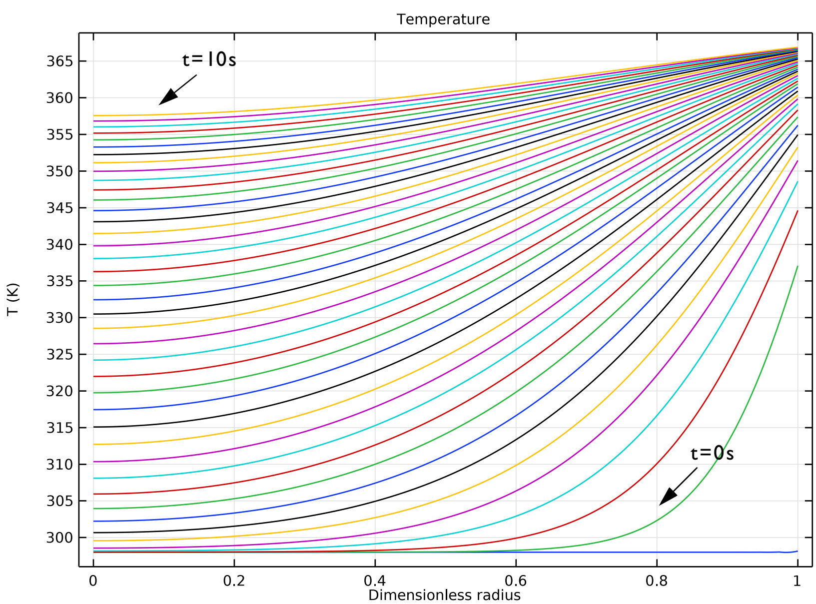


Figure 2: Temperature profiles from t = 0 to t = 10 s.

Figure 2 shows the temperature profiles from 0 to 10 seconds. Each line represents an increment of 0.5 s from the preceding line. From the topmost line it is clear that the center of the pellet has not reached steady state at 10 s. You can also plot the time evolution of the temperature at the center of the pellet.

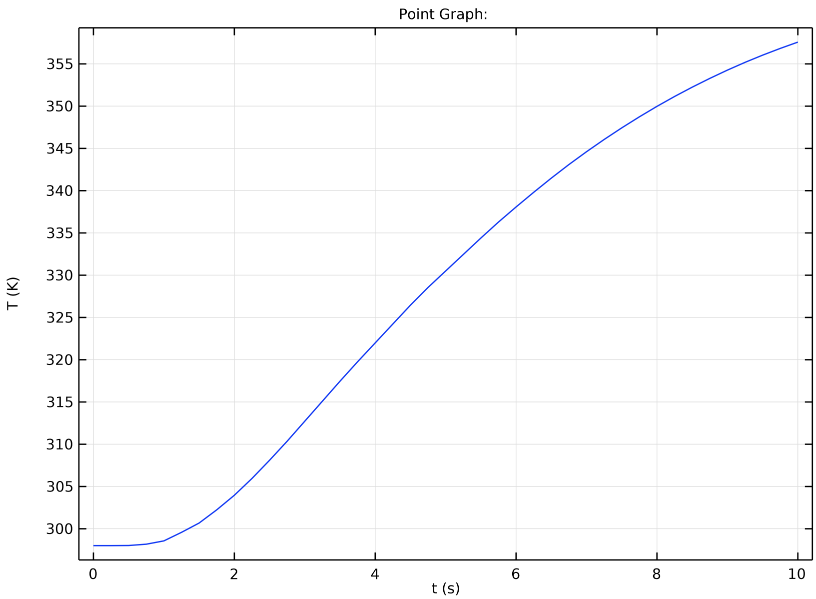


Figure 3: Time evolution of temperature in the center of a pellet with radius $R_p = 5$ mm.

Figure 3 shows even more clearly how long the process must yet go before it reaches steady state. An interesting next step is to experiment with different particle radii, R_p, and different heating times.

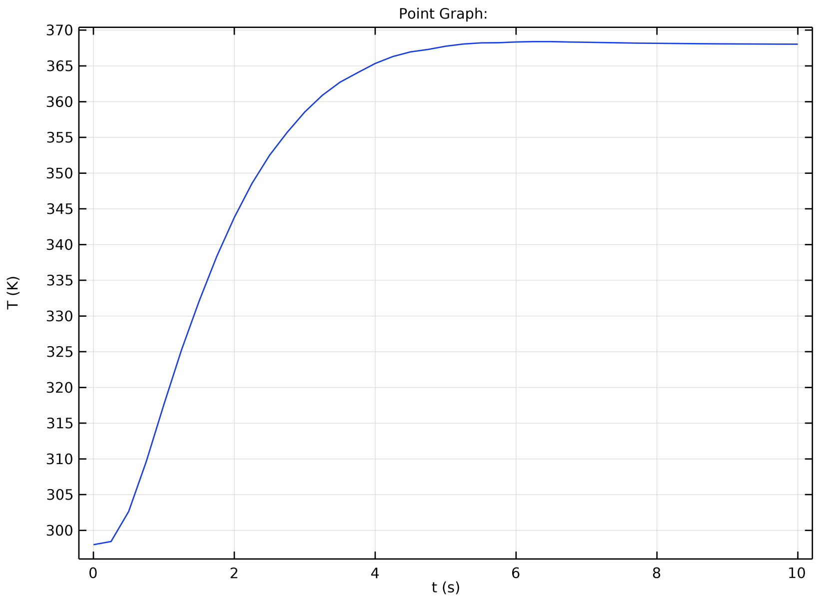


Figure 4: Time evolution in the center of a pellet with radius R_p = 2.5 mm.

Simply reducing the radius somewhat lets the model reach steady state within 7 s.

Notes About the COMSOL Implementation

To implement Equation 2 and the boundary conditions of this problem, use the 1D time-dependent version of the General Form PDE interface:

$$\begin{cases} e_a\dfrac{\partial^2 u}{\partial t^2}+d_a\dfrac{\partial u}{\partial t}+\nabla\cdot\Gamma=F & \text{in }\Omega \\ -\mathbf{n}\cdot\Gamma=G+\left(\dfrac{\partial R}{\partial u}\right)^T\mu & \text{on }\partial\Omega \\ 0=R & \text{on }\partial\Omega \end{cases}$$

The space coordinate in the model is $\hat{r}$. For typographical reasons we use rh in this model for “r-hat.” Identifying the general form with Equation 2, the following settings generate the correct equation:

COEFFICIENT	EXPRESSION
e_a	0
d_a	$\hat{r}^2 \rho c_p$
Γ (flux vector)	$\frac{-k\hat{r}^2}{R_p^2}\frac{\partial T}{\partial \hat{r}}$
F (source term)	0

You must take special care when setting the heat-influx boundary condition on the pellet surface. $h_s(T_{\mathrm{ext}} - T) = k\partial T/\partial r$ on the surface, so you need to compensate G accordingly:

$$G = \frac{\hat{r}^2}{R_p} h_s(T_{\mathrm{ext}} - T)$$

Application Library path: `COMSOL_Multiphysics/Equation_Based/spherically_symmetric_transport`

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 **Mathematics>PDE Interfaces>General Form PDE (g)**.

3 Click **Add**.

4 In the **Dependent variables** table, enter the following settings:

T

5 Click **Study**.

6 In the **Select Study** tree, select **General Studies>Time Dependent**.

7 Click **Done**.

ROOT

1 In the **Model Builder** window, click the root node.

2 In the root node's **Settings** window, locate the **Unit System** section.

3 From the **Unit system** list, choose **None**.

The equations in this model are given using the dimensionless radial coordinate. Turning off unit support avoids warnings about inconsistent use of units.

GLOBAL DEFINITIONS

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
rho	2000	2000	Density (kg/m^3)
cp	300	300	Heat capacity (J/(kg*K))
k	0.5	0.5	Thermal conductivity (W/(m*K))
Rp	0.005	0.005	Pellet radius (m)
Qs	0	0	Heat source (W/m^3)
hs	1000	1000	Heat transfer coefficient (W/(m^2*K))
Text	368	368	External temperature (K)
Tinit	298	298	Initial value (K)

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**, click **Build All Objects**.

GENERAL FORM PDE (G)

General Form PDE 1

1 In the **Model Builder** window, under **Component 1 (comp1)>General Form PDE (g)** click **General Form PDE 1**.

2 In the **Settings** window for **General Form PDE**, locate the **Conservative Flux** section.

3 In the Γ text field, type `-k*x^2/Rp^2*Tx`.

4 Locate the **Source Term** section. In the f text field, type `x^2*Qs`.

5 Locate the **Damping or Mass Coefficient** section. In the d_a text field, type `x^2*rho*cp`.

Note that `Tx` is the COMSOL Multiphysics syntax for the partial derivative of the variable T with respect to the coordinate x.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the T text field, type `Tinit`.

Flux/Source 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Flux/Source**.

2 Select Boundary 1 only.

Flux/Source 2

1 In the **Physics** toolbar, click **Boundaries** and choose **Flux/Source**.

2 Select Boundary 2 only.

3 In the **Settings** window for **Flux/Source**, locate the **Boundary Flux/Source** section.

4 In the g text field, type `x^2/Rp*hs*(Text-T)`.

MESH 1

Scale 1

1 In the **Mesh** toolbar, click **More Attributes** and choose **Scale**.

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

3 In the **Element size scale** text field, type `0.4`.

Edge 1

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

2 In the **Settings** window for **Edge**, click **Build All**.

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. In the **Output times** text field, type `range(0,0.25,10)`.
4. In the **Home** toolbar, click **Compute**.

RESULTS

The default plot shows the temperature versus the dimensionless radius for all times in the specified interval.

1D Plot Group 1

1. In the **Model Builder** window, under **Results** click **1D Plot Group 1**.
2. In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.
3. From the **Title type** list, choose **Manual**.
4. In the **Title** text area, type `Temperature`.
5. Locate the **Plot Settings** section.
6. Select the **x-axis label** check box. In the associated text field, type `Dimensionless radius`.
7. Select the **y-axis label** check box. In the associated text field, type `T (K)`.
8. In the **1D Plot Group 1** toolbar, click **Plot**.

To plot the time evolution of temperature at the center of the pellet of radius 5 mm (Figure 3), follow the steps given below.

1D Plot Group 2

In the **Home** toolbar, click **Add Plot Group** and choose **1D Plot Group**.

Point Graph 1

1. Right-click **1D Plot Group 2** and choose **Point Graph**.
2. Select Boundary 1 only.

1D Plot Group 2

1. In the **Model Builder** window, click **1D Plot Group 2**.
2. In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.
3. Select the **x-axis label** check box. In the associated text field, type `t (s)`.
4. Select the **y-axis label** check box. In the associated text field, type `T (K)`.

5 In the **1D Plot Group 2** toolbar, click **Plot**.

Now change the pellet radius to 2.5 mm in the **Parameters** section and see its effect on the time evolution of temperature at the center of the pellet.

GLOBAL DEFINITIONS

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
`Rp`	`0.0025`	0.0025	`Pellet radius (m)`

STUDY 1

In the **Home** toolbar, click **Compute**.

RESULTS

1D Plot Group 2

The resulting plot should look like Figure 4.

1 In the **Model Builder** window, under **Results** click **1D Plot Group 2**.

2 In the **1D Plot Group 2** toolbar, click **Plot**.