

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 heatconduction 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

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

where ρ is the density (kg/m³), c_p gives the heat capacity (J/(kg·K)), k denotes the thermal conductivity $(W/(m \cdot K))$, 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

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

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

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

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 size¹. 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:

$$\hat{r}=0$$
 $\hat{r}=1$

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)
$R_{ m p}$	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/(m²·K)), for the influx of heat (W/m²):

$$q_{\rm in} = h_{\rm s}(T_{\rm ext} - T)$$

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

Results

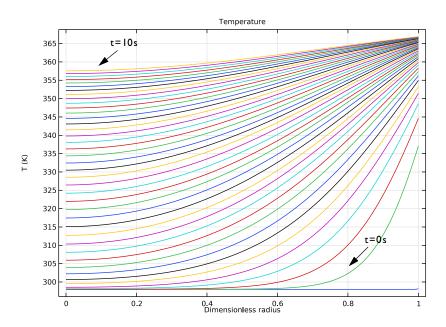


Figure 2: Temperature profiles from t = 0 to t = 10 s.

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.

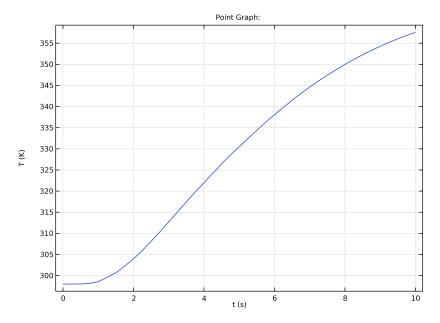


Figure 3: Time evolution of temperature in the center of a pellet with radius $R_p = 5$ mm.

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.

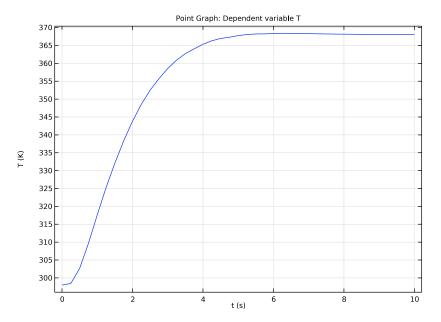


Figure 4: Time evolution in the center of a pellet with radius $R_p = 2.5$ mm.

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 timedependent version of the General Form PDE interface:

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

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	$\hat{r}^2 ho c_p$
Γ (flux vector)	$rac{-k\hat{r}^2}{R_p^2}rac{\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. $h_s(T_{\text{ext}} - T) = k \partial T / \partial r$ on the surface, so you need to compensate G accordingly:

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

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

- I In the Model Wizard window, click ID.
- 2 In the Select Physics tree, select Mathematics>PDE Interfaces>General Form PDE (g).
- 3 Click Add.
- 4 In the **Dependent variables (1)** table, enter the following settings:

Т

- 5 Click Study.
- 6 In the Select Study tree, select General Studies>Time Dependent.
- 7 Click M Done.

ROOT

- I 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

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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)
ср	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 I

Interval I (iI)

- I In the Model Builder window, under Component I (compl) right-click Geometry I and choose Interval.
- 2 In the Settings window for Interval, click **Build All Objects**.

GENERAL FORM PDE (G)

General Form PDE 1

- I In the Model Builder window, under Component I (compl)>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 .
- **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

- I In the Model Builder window, click Initial Values I.
- 2 In the Settings window for Initial Values, locate the Initial Values section.
- **3** In the *T* text field, type Tinit.

Flux/Source 1

- I In the Physics toolbar, click Boundaries and choose Flux/Source.
- 2 Select Boundary 1 only.

Flux/Source 2

- I 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 I

Scale 1

- I In the Mesh toolbar, click A 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 I

- I In the Mesh toolbar, click A Edge.
- 2 In the Settings window for Edge, click Build All.

STUDY I

Step 1: Time Dependent

- I In the Model Builder window, under Study I click Step I: 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.

General Form PDE

- I In the Model Builder window, under Results click General Form PDE.
- 2 In the Settings window for ID 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 General Form PDE 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.

ID Plot Group 2

In the Home toolbar, click Add Plot Group and choose ID Plot Group.

Point Grabh 1

- I Right-click ID Plot Group 2 and choose Point Graph.
- 2 Select Boundary 1 only.

ID Plot Group 2

- I In the Model Builder window, click ID Plot Group 2.
- 2 In the Settings window for ID 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 ID 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

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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 I

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

RESULTS

ID Plot Group 2

The resulting plot should look like Figure 4.

- I In the Model Builder window, under Results click ID Plot Group 2.
- 2 In the ID Plot Group 2 toolbar, click Plot.