Created in COMSOL Multiphysics 6.2

Parameter Estimation for Pyrolysis of Wood

Introduction

The process of pyrolyzing wood to produce tar and charcoal has been important since ancient times. Tar was used to impregnate wood for ships, and char was essential for iron smelting. Material for both of these applications have later been replaced by fossil sources, but environmental concerns has since kindled the interest for products produced by pyrolyzing wood.

Pyrolysis is thermal decomposition in the absence of an oxidizing atmosphere. In other words; heat something up without air until it decomposes. Historically, tar and charcoal were produced in piles, or pits, where wood was covered with for example dirt to prevent air from reaching the inside of the pile. The wood was lit on fire and allowed to smolder, but not burn (combust). During smoldering (pyrolysis), volatile species, water, and light decomposition products, leave the solid, resulting in charcoal. In modern times, steel reactors with an inert atmosphere are used.

The products that result from pyrolysis will depend on the feedstock type and particle size, the heating rate, the final temperature, and the duration of the process. Due to the complexity of the reaction mechanism, so called lumped-reaction models are often used. The reaction products are lumped into pseudo species based on their phase, which gives a simplified reaction scheme that can be used for engineering purposes. One such reaction scheme is seen in Figure 1.

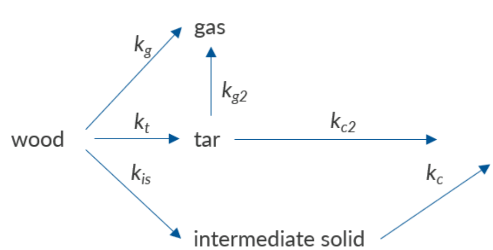

Figure 1: The reaction scheme used in this model consists of four pseudo species, namely gas (g), tar (t), intermediate solid (is), and char (c).

The scheme was proposed by Park and others (Ref. 1) to describe the pyrolysis of a wooden sphere, approximately 1 cm in diameter, inserted into a hot furnace. The experimental setup is illustrated in Figure 2.

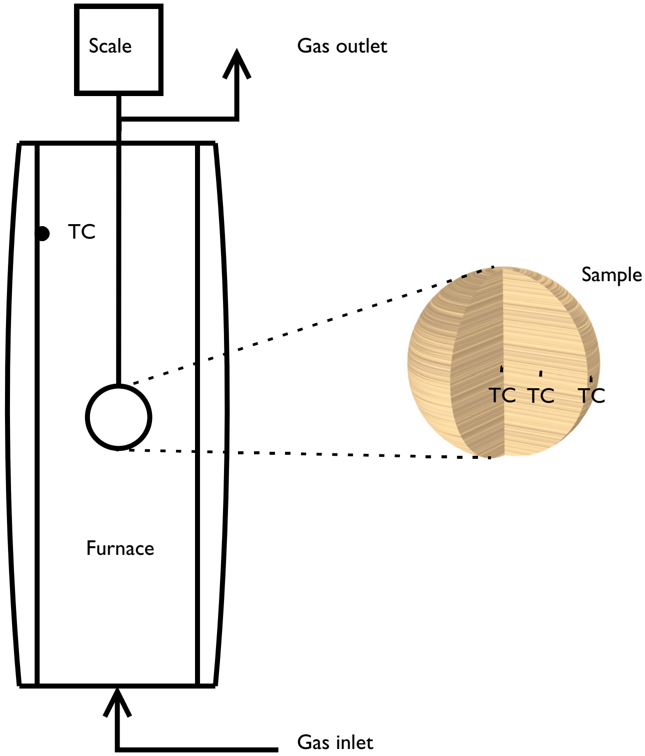

Figure 2: The experimental system setup consists of an isothermal furnace with inert atmosphere, a sample holder attached to a scale, and thermocouples (TC) measuring the temperature of the system. The sample radius is approximately 1 cm.

The experimental system consists of an isothermal furnace with inert atmosphere. The temperature of the furnace, measured by thermocouples (TC), is kept constant, and the inert atmosphere is achieved by nitrogen flowing through the furnace chamber. For each experiment, the sample is inserted into the isothermal furnace, and the sample temperature and the sample mass are recorded during the pyrolysis process. The temperature gradient within the sample is significant and the temperature is thus measured at three positions within the sample; at the surface, mid and center position. Wood is a porous, anisotropic material and in this study the temperature was measured along the fibers in the horizontal direction.

The reaction scheme in Figure 1 describes both primary and secondary pyrolysis reactions. The primary decomposition steps will convert wood into the pseudo species gas, tar, and intermediate solid. Gaseous species are those that do not condense at room temperature, for example carbon monoxide. Tar species are all the condensable volatiles, for example water, carboxylic acids and phenols. The gases and the tars leaving the particle result in mass loss. On its way out from the porous particle, the tar may decompose to form gas or char. The intermediate solid further converts into char.

Experimental results from Ref. 1 showing development of the sample mass and the temperature are shown in Figure 3.

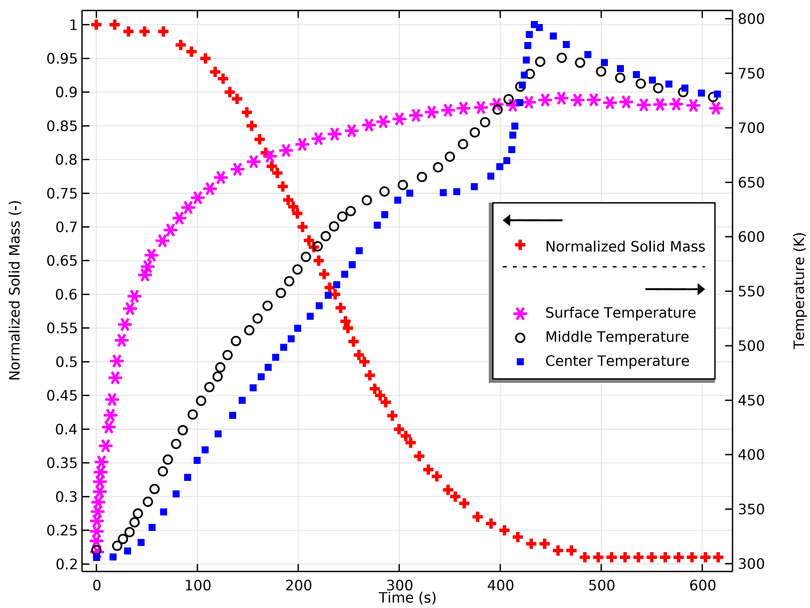

Figure 3: Experimental data from Ref. 1. The mass has been normalized by the initial sample mass.

This example model, based on Ref. 1 and Ref. 2, consists of two parts. The first part demonstrates how to set up a model describing the pyrolysis process, heat, and momentum transfer in an anisotropic wood sphere. In the last part, parameter estimation is used to optimize the model using the experimental data in Figure 3. The parameters to be estimated are one Arrhenius constant, two reaction heats, and one external heat transfer coefficient (see Table 1).

Model Definition

The pyrolysis of a centimeter-sized wood particle presents a fully coupled multiphysics problem with mass transfer, fluid flow and heat transfer. In this example, both the conductive heat transfer and the permeability of the solid are anisotropic.

MASS TRANSPORT

The pyrolysis reaction scheme in Figure 1 consists of gaseous and solid species. The reaction rate expressions ($\mathrm{kg/(m^3{\cdot}s)}$), for the solid species wood (w), intermediate solid (is), and char (c) are expressed in terms of their respective density in the manner of

$$\frac{\partial \rho_{\mathrm{w}}}{\partial t} = -(k_{\mathrm{t}} - k_{\mathrm{g}} - k_{\mathrm{is}})\rho_{\mathrm{w}}, \tag{1}$$

$$\frac{\partial \rho_{\mathrm{is}}}{\partial t} = k_{\mathrm{is}}\rho_{\mathrm{w}} - k_{\mathrm{c}}\rho_{\mathrm{is}}, \tag{2}$$

and

$$\frac{\partial \rho_{\mathrm{c}}}{\partial t} = k_{\mathrm{c}}\rho_{\mathrm{is}} + k_{\mathrm{c2}}\rho_{\mathrm{t}}. \tag{3}$$

The density is defined as the bulk density of the solid, and thus includes the porosity ε of the solid domain. k_i is the Arrhenius rate constant ($1/\mathrm{s}$), as indicated in the reaction scheme (Figure 1)

$$k_i = A_i \exp(-E_i/(RT)). \tag{4}$$

No transport terms are needed for the solid species, and Equation 1-3 are thus sufficient to conserve the mass of the solid species.

The mass conservation equation for the gas species i includes diffusion, convection, and the reaction rate terms. The gas mixture inside the particle consists solely of gas, tar, and inert gas, the mass balance is expressed in terms of the respective mass fractions ω as

$$\varepsilon\rho\frac{\partial \omega_i}{\partial t} + \nabla\cdot\mathbf{j}_i + \rho(\mathbf{u}\cdot\nabla)\omega_i = R_i. \tag{5}$$

Here, ρ is the density of the fluid in the pores, derived using the ideal gas law, and ε is the porosity of the porous domain:

$$\varepsilon = 1 - \frac{\rho_{\mathrm{w}} + \rho_{\mathrm{is}} + \rho_{\mathrm{c}}}{\rho_{\mathrm{w},0}}(1 - \varepsilon_{\mathrm{w0}}).$$

The initial wood porosity, $\varepsilon_{\mathrm{w0}}$, is 0.4.

In Equation 5, $\mathbf{j}_i$ is the diffusional flux as described by Fick's law, with diffusion coefficients D_i, and a Millington and Quirk model to derive the effective diffusivity:

$$\mathbf{j}_i = -\rho\left(\varepsilon^{4/3} D_i \nabla\omega_i - \omega_i \sum_k D_k \nabla\omega_k\right),$$

The mass averaged velocity of the mixture in the pores, $\mathbf{u}$, is derived using Darcy's law:

$$\mathbf{u} = -\frac{\kappa}{\mu}\nabla p\,. \tag{6}$$

Here, μ is the viscosity (kg/(m·s)), p is the pressure (Pa), and κ is the effective permeability (m^2);

$$\kappa_j = \frac{\rho_{\mathrm{w}}\kappa_{\mathrm{w},j} + (\rho_{\mathrm{is}} + \rho_{\mathrm{c}})\kappa_{\mathrm{c},j}}{\rho_{\mathrm{w}} + \rho_{\mathrm{is}} + \rho_{\mathrm{c}}},$$

where j indicates *across* or *along* the fiber direction.

The reaction rate expressions for the gas phase species tar (t) and gas (g) are:

$$R_{\mathrm{t}} = \rho\frac{\partial\omega_{\mathrm{t}}}{\partial t} = k_{\mathrm{t}}\rho_{\mathrm{w}} - k_{\mathrm{c2}}\rho\omega_{\mathrm{t}} - k_{\mathrm{g2}}\rho\omega_{\mathrm{t}},$$

and

$$R_{\mathrm{g}} = \rho\frac{\partial\omega_{\mathrm{g}}}{\partial t} = k_{\mathrm{g}}\rho_{\mathrm{w}} + k_{\mathrm{g2}}\rho\omega_{\mathrm{t}}.$$

Mass transfer through the exterior boundary of the particle is dominated by convection. A boundary condition assuming no diffusive flux is thus applicable;

$$-\mathbf{n}\cdot\mathbf{j}_i = 0.$$

Here, $\mathbf{n}$ denotes the outward pointing normal of the exterior boundary.

MOMENTUM TRANSPORT

The fluid flow is defined with the continuity equations

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = Q_{\mathrm{m}},$$

with a Darcian flow (see Equation 6), and a mass source term (evolution of fluid species) defined as

$$Q_{\mathrm{m}} = k_{\mathrm{t}}\rho_{\mathrm{w}} - k_{\mathrm{c2}}\rho\omega_{\mathrm{t}} + k_{\mathrm{g}}\rho_{\mathrm{w}}. \tag{7}$$

At the exterior boundary, a zero relative pressure with respect to the reference pressure ($p_{\mathrm{ref}} = 1$ atm) is prescribed;

$$p = 0.$$

HEAT TRANSPORT

The energy balance equation applied to the fluid (f) in the pores, and the solid bulk (b) of the wood sample assumes local thermal equilibrium, and considers heat transfer through convection, radiation, and conduction:

$$(\rho C_p)_{\mathrm{eff}}\frac{\partial T}{\partial t} + \nabla \cdot (-k_{\mathrm{eff}}\nabla T) + \rho_{\mathrm{f}} C_{\mathrm{p,f}}(\mathbf{u} \cdot \nabla)T = Q. \tag{8}$$

Here, Q is the heat of reaction

$$Q = -\rho_{\mathrm{w}}(k_{\mathrm{t}}\Delta H_{\mathrm{t}} + k_{\mathrm{g}}\Delta H_{\mathrm{g}} + k_{\mathrm{is}}\Delta H_{\mathrm{is}}) - \rho_{\mathrm{is}}k_{\mathrm{c}}\Delta H_{\mathrm{c}} - \rho_{\mathrm{t}}k_{\mathrm{g2}}\Delta H_{\mathrm{g2}} - \rho_{\mathrm{t}}k_{\mathrm{c2}}\Delta H_{\mathrm{c2}}. \tag{9}$$

In Equation 8 $(\rho C_p)_{\mathrm{eff}}$ is defined as

$$(\rho C_{\mathrm{p}})_{\mathrm{eff}} = \varepsilon\rho_{\mathrm{f}} C_{\mathrm{p,f}} + \rho_{\mathrm{b}} C_{\mathrm{p,b}}.$$

The heat capacities at constant pressures for the fluid and bulk phases are

$$C_{\mathrm{p,f}} = \omega_{\mathrm{t}} C_{\mathrm{p,t}} + \omega_{\mathrm{N2}} C_{\mathrm{p,N2}} + \omega_{\mathrm{g}} C_{\mathrm{p,g}},$$

and

$$C_{\mathrm{p,b}} = \frac{(C_{\mathrm{p,w}}\rho_{\mathrm{w}} + C_{\mathrm{p,c}}(\rho_{\mathrm{is}} + \rho_{\mathrm{c}}))}{\rho_{w,0}}.$$

The dry bulk density ρ_{b} is $(1 - \varepsilon)\rho_{\mathrm{w,0}}$ and the fluid density ρ_{f} is derived from the ideal gas law.

The effective thermal conductivity is the weighted sum of the conductivity of the fluid, k_{f}, of the solid bulk, k_{b}, as well as a contribution from the radiation in the pores;

$$k_{\text{eff}} = \varepsilon k_{\text{f}} + k_{\text{b}} + \varepsilon \frac{13.5\sigma T^3 d_{\text{eff}}}{e},$$

where σ is the Boltzmann constant ($\text{W}/(\text{m}^2\cdot\text{K}^4)$), and e is the emissivity. d_{eff} is the effective pore diameter (m), Defined as the weighted sum of the pore diameter in the wood and the char

$$d_{\text{eff}} = d_{\text{w}}(1-\eta) + d_{\text{c}}\eta.$$

The degree of pyrolysis, η is

$$\eta = 1 - \frac{(\rho_{\text{w}} + \rho_{\text{is}})}{\rho_{\text{w},0}}.$$

The conductivity of the solid bulk is anisotropic

$$k_{b,j} = \frac{\rho_{\text{w}} k_{\text{w},j} + (\rho_{\text{is}} + \rho_{\text{c}}) k_{\text{c},j}}{\rho_{\text{w}} + \rho_{\text{is}} + \rho_{\text{c}}},$$

where j indicates *across* or *along* the fiber direction.

The external boundary of the particle has a heat flux boundary condition;

$$-\mathbf{n} \cdot \mathbf{q} = q_0,$$

where the heat flux q_0 is the sum of convective and radiative heat flux:

$$q_0 = h_{\text{conv}}(T_{\text{gas}} - T) + \sigma e_s({T_{\text{reactor}}}^4 - T^4). \tag{10}$$

Here, h_{conv} is the heat transfer coefficient in the gas surrounding the particle, T_{gas} is the gas temperature in the reactor, σ is the Stefan–Boltzmann constant, e_{s} is the surface emissivity, T_{reactor} is the reactor temperature, and T is the surface temperature of the sample. All temperatures are expressed in K.

PARAMETER ESTIMATION

Parameter estimation problems consist of three components: (i) experimental data; (ii) a forward model that represents the physics of the experiments; and (iii) an optimization algorithm that compares the two and updates the model parameters to minimize the difference. This can be formulated mathematically as a nonlinear least-squares minimization problem,

$$\mathbf{q}_{\text{opt}} = \operatorname{argmin}_{\mathbf{q}}\left(\sum_{n=1}^{N} Q_n\right) \tag{11}$$

with

$$Q_n = \frac{1}{2}\sum_{m=1}^{M_n} (P_n(\mathbf{u}(\mathbf{q}), \mathbf{q}) - \hat{P}_{nm})^2 \tag{12}$$

Herein, $\mathbf{q}$ is the vector of control parameters (ξ) that we want to estimate, N is the number of experiments, M_n is the number of data points per experiment, $\hat{P}_{nm}$ is the mth data point of experiment n, and $P_n(\mathbf{u}(\mathbf{q}), \mathbf{q})$ denotes the corresponding model prediction given the PDE solution $\mathbf{u}$.

In this example, we consider $N = 4$ experimental data sets from Ref. 1 (see Figure 3), for which the measured quantity P_n is either the temperature (at one of the thermocouple positions, see Figure 2) or the normalized solid mass, and $\mathbf{u}$ is the solution to the multiphysics model set up to describe the system.

The normalized solid mass Y is defined as

$$Y = \frac{\rho_{\text{w}} + \rho_{\text{is}} + \rho_{\text{c}}}{\rho_{\text{w},0}}. \tag{13}$$

In this model, the control parameters to estimate are $\mathbf{q} = (A_{\text{is}}, \Delta H_{\text{t}}, \Delta H_{\text{c}}, h_{\text{conv}})$, where A_{is} is the Arrhenius frequency factor for the primary pyrolysis step where wood turns to intermediate solid (Equation 4). ΔH_{t} and ΔH_{c} are the heat of reaction for formation of tar from wood, and formation of char from intermediate solid (Equation 9). In this model the primary reactions all share the same heat of reactions, namely $\Delta H_{\text{t}} = \Delta H_{\text{g}} = \Delta H_{\text{is}}$. The final control parameter h_{conv} is the convective heat transfer coefficient external to the particle (Equation 10). The parameters along with the initial guess of their values are provided in Table 1.

TABLE 1: PARAMETERS TO ESTIMATE AND THEIR INITIAL VALUES

Parameter	**Name**	**Initial guess**
Arrhenius frequency factor wood -> intermediate solid	A_is	1e7[1/s]
Heat of reaction wood -> tar	DH_t	-200[kJ/kg]

TABLE 1: PARAMETERS TO ESTIMATE AND THEIR INITIAL VALUES

Parameter	Name	Initial guess
Heat of reaction intermediate solid -> char	DH_c	50[kJ/kg]
Convective heat transfer coefficient	hconv	5[W/m^2/K]

Results and Discussion

The results from the forward model, using the initial guess of the parameter values in Table 1, are shown in Figure 4 and Figure 5. The model describes the trends in the temperatures and solid mass quite well, especially for the middle temperature (Figure 5). Both the timings and the absolute values of the peak temperatures for each position are lower than in experiments, and the experimental final solid mass is not captured by the model at all.

The model predictions after parameter estimation are illustrated in Figure 6 and Figure 7. For comparison, the results from the forward model are also included in those figures. It is clear that the optimized model better predicts the experimental results. The timing of the center temperature peak, and its value, is now captured, and so is the final solid mass.

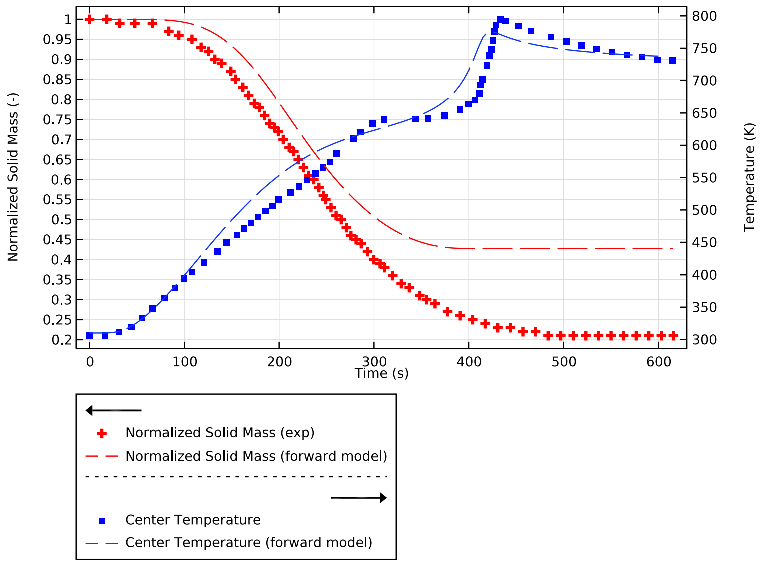

Figure 4: Normalized solid mass, and center temperature, using initial values of the control parameters.

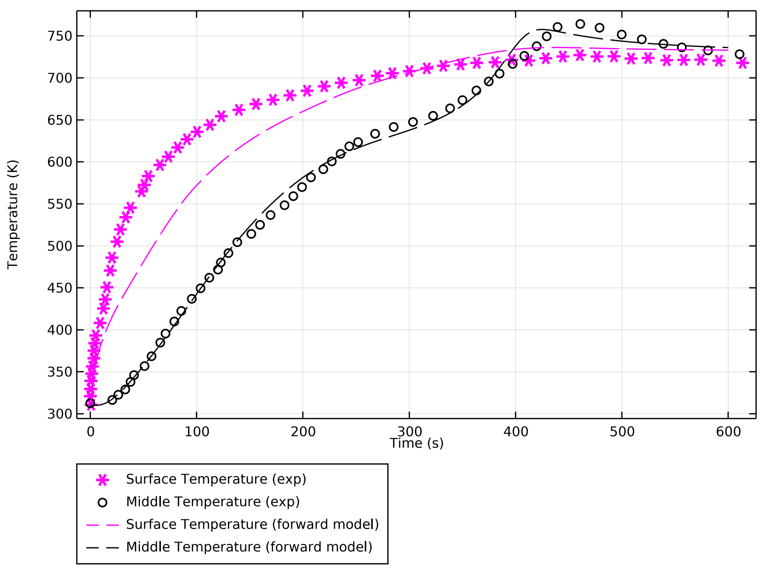

Figure 5: Surface, and middle temperatures, using initial values of the control parameters.

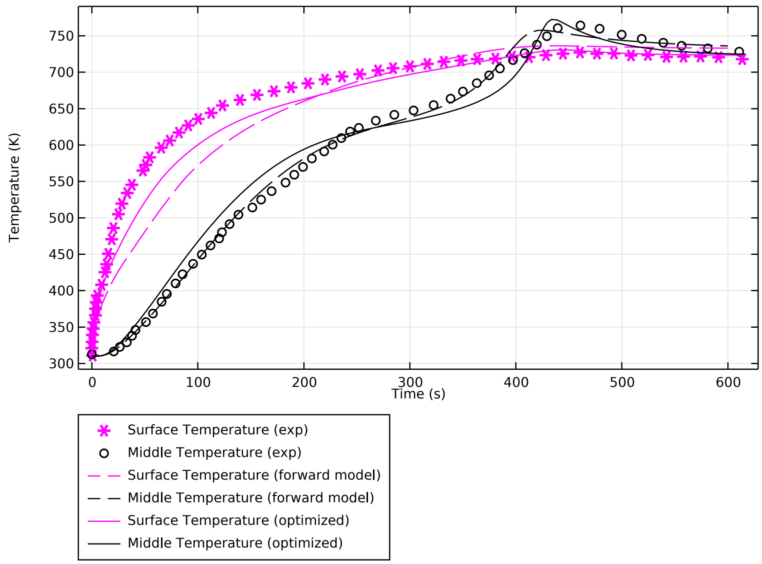

Figure 6: Surface and middle temperatures from the forward and the optimized model.

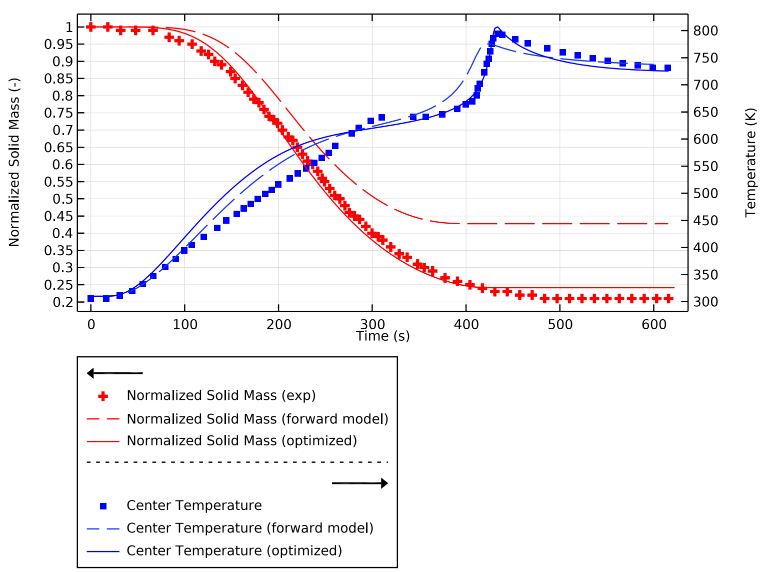

Figure 7: Center temperature and normalized solid mass from the forward and optimized model.

[Figure 8](#) illustrates the changes in solid composition in the particle at three different times. Early in the process, there is mainly wood. This wood is converted into gases and the solid intermediate species (is). Late in the process, the wood is fully converted, and most of the particle consists of char.

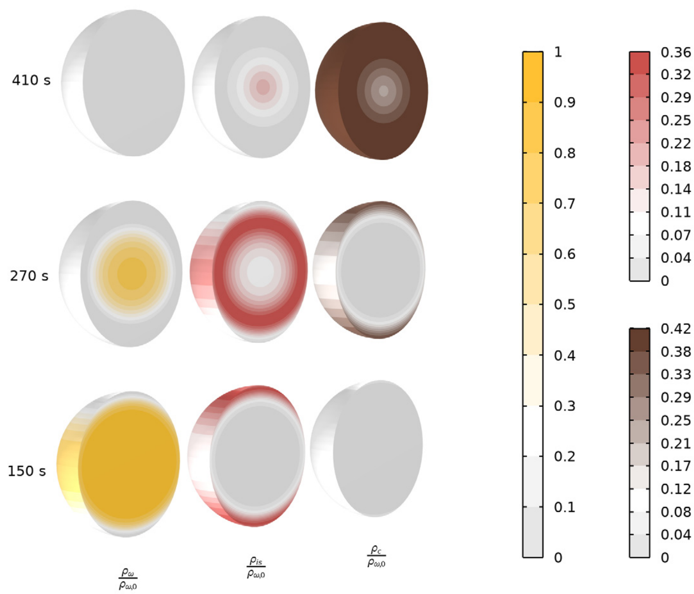

Figure 8: Normalized densities of wood $\rho_w/\rho_{w,0}$*, intermediate solid* $\rho_{is}/\rho_{w,0}$*, and char* $\rho_c/\rho_{w,0}$*, at three different times.*

Figure 6 and Figure 7 above show the temperatures at the thermocouple positions in the particle. Figure 9 - Figure 11 illustrate the temperature in the solid domain, together with both the mass source (Q_m in Equation 7) and the heat source (Q in Equation 9). As expected, at an early stage (Figure 9), a positive mass source is accompanied with a negative heat source, since the primary pyrolysis reactions, producing gaseous species, are endothermic.

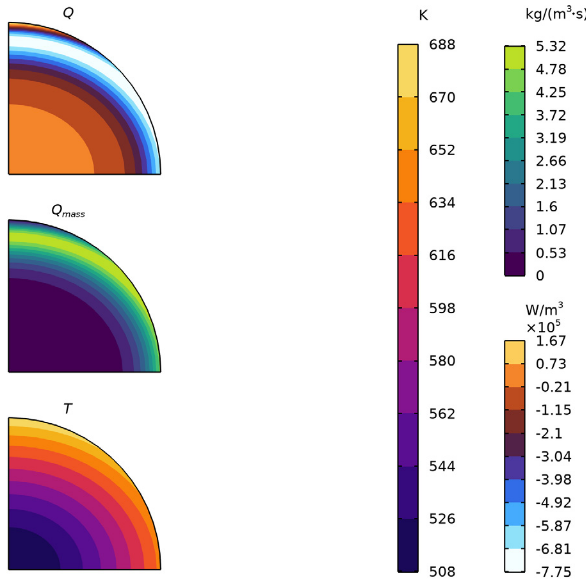

Figure 9: Temperature, mass source, and heat source in the modeled geometry, 150 s into the pyrolysis process.

As the process progresses (Figure 10), a negative mass source and a positive heat source is seen, indicating the formation of char. This is also seen in Figure 8.

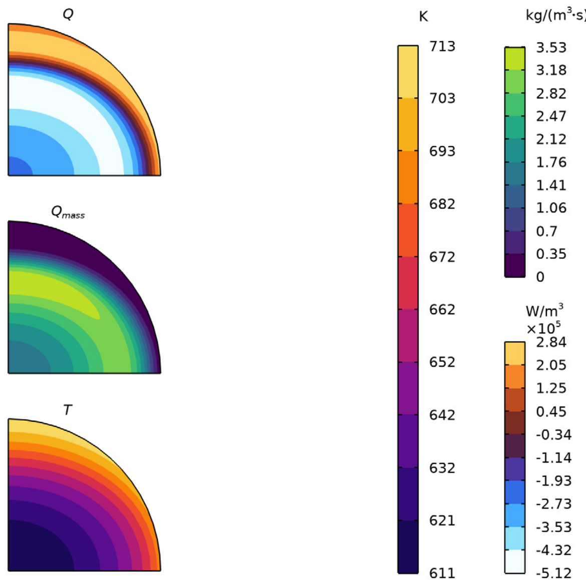

Figure 10: Temperature, mass source, and heat source in the modeled geometry, 270 s into the pyrolysis process.

At the last stage of the mass loss process, depicted in Figure 11, there are no gas forming reactions, and only exothermic processes, as seen by a negative mass source and a positive heat source.

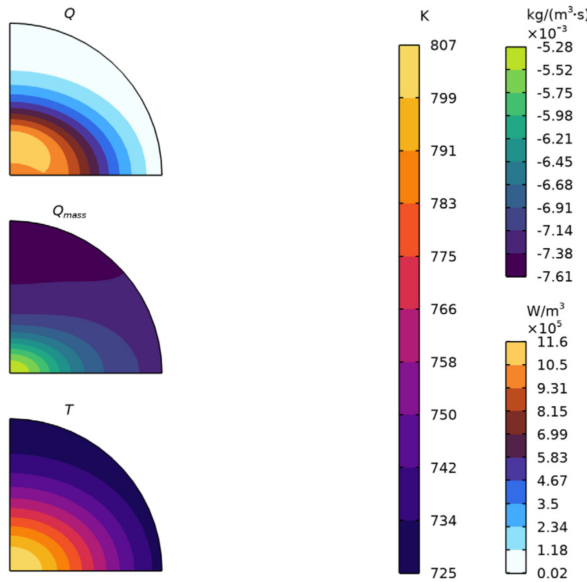

Figure 11: Temperature, mass source, and heat source in the modeled geometry, 433 s into the pyrolysis process. This time corresponds to the temperature peak seen in Figure 7.

One thing seen in Figure 8-Figure 11 is the anisotropic particle properties. Figure 12 illustrates this further by showing the relative pressure in the particle, p/p_{ref}, the total Darcy velocity magnitude, U, the Darcy velocity vector, $\mathbf{u}$, the porosity, ε, and the solid mass fraction, Y (see Equation 13).

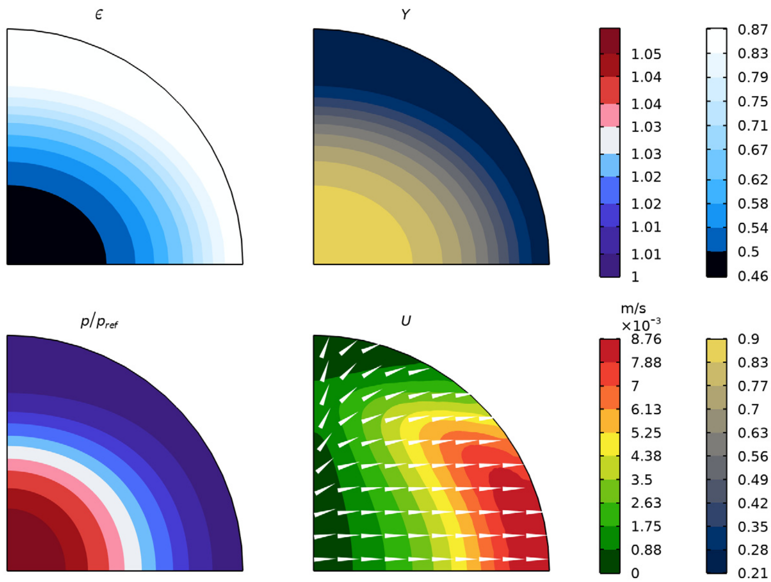

Figure 12: The relative pressure in the particle, p/p_{ref}, the total Darcy velocity magnitude, U, the Darcy velocity, $\mathbf{u}$, the porosity, ε, and the solid mass fraction, Y.

Notes About the COMSOL Implementation

The solid phase reactions in Figure 1 are implemented in the **Domain ODEs and DAEs** interface.

In parameter estimation problems, it is good practice to first set up and test the forward model before solving the inverse problem.

The **Parameter Estimation** functionality is available in COMSOL Multiphysics in the context menu of a **Component** or under **Optimization** in the **Physics** toolbar, wherein each **Global Least-Squares Objective** node adds an objective corresponding to Equation 12 to the model. To solve the inverse problem, these need to be combined with a study containing a **Parameter Estimation** study step. When multiple objectives are selected in the study step, the total objective function that is minimized will be the sum of all objectives selected, see Equation 11. For most least-squares problems, the **Levenberg–Marquardt** algorithm with a finite difference approximation of the Jacobian is a robust and efficient choice of optimization solver. If the gradient cannot be derived analytically, or is time consuming to evaluate numerically, then a gradient-free algorithm like the **BOBYQA** is needed. To increase the stability of the optimization process, the logarithm of the control parameters can be optimized. This gives scales of 1, and initial values equal to zero. This strategy is used in this example model.

References

1. W.C. Park, A. Atreya, and H.R. Baum, "Experimental and theoretical investigation of heat and mass transfer processes during wood pyrolysis," *Combustion and Flame*, vol. 157, pp. 481–494, 2010.

2. X. Shi, F. Ronsse, and J.G. Pieters, "Finite element modeling of intraparticle heterogeneous tar conversion during pyrolysis of woody biomass particles," *Fuel Processing Technology*, vol. 148, pp. 302-316, 2016.

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/parameter_estimation_pyrolysis_wood`

Modeling Instructions

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

NEW

1. In the **New** window, This model consists of two parts: setting up the forward model and performing parameter estimation to calibrate that model with experimental data. Start by setting up the forward model.

   Use the **Model Wizard** to add a Component (2D axisymmetric due to the anisotropic sphere); the physics **Darcy's Law**, **Transport of Concentrated Species in Porous Media**, **Heat Transfer in Porous Media**, and **Domain ODEs and DAEs** (for the solid reactions); and a **Time Dependent** study to follow the decomposition progress.
2. click **Model Wizard**.

MODEL WIZARD

1. In the **Model Wizard** window, click **2D Axisymmetric**.
2. In the **Select Physics** tree, select **Chemical Species Transport> Transport of Concentrated Species in Porous Media (tcs)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Fluid Flow>Porous Media and Subsurface Flow> Darcy's Law (dl)**.

5 Click **Add**.

6 In the **Select Physics** tree, select **Heat Transfer>Porous Media> Heat Transfer in Porous Media (ht)**.

7 Click **Add**.

8 In the **Select Physics** tree, select **Mathematics>ODE and DAE Interfaces> Domain ODEs and DAEs (dode)**.

9 Click **Add**.

10 Click **Study**.

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

12 Click **Done**.

Before setting up the geometry, load all the parameters and variables for this model from files. Since we have not yet defined the physics, some of the expressions in the variable files will be undefined at this point.

GLOBAL DEFINITIONS

Sample Properties

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

2 In the **Settings** window for **Parameters**, type `Sample Properties` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

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

Experimental Conditions

1 In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type `Experimental Conditions` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

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

Reaction Parameters

1 In the **Home** toolbar, click **Pi Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type `Reaction Parameters` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

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

DEFINITIONS

Solid Species Variables

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

2 In the **Settings** window for **Variables**, type `Solid Species Variables` in the **Label** text field.

3 Locate the **Variables** section. Click **Load from File**.

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

Reaction Variables

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Reaction Variables` in the **Label** text field.

3 Locate the **Variables** section. Click **Load from File**.

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

Fluid Species Variables

1 Right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `Fluid Species Variables` in the **Label** text field.

3 Locate the **Variables** section. Click **Load from File**.

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

External Boundary Variables

1 Right-click **Definitions** and choose **Variables**.

2 In the **Settings** window for **Variables**, type `External Boundary Variables` in the **Label** text field.

3 Locate the **Variables** section. Click the **Load** button. From the menu, choose **Load from File**.

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

Set up the geometry. It consists of a 1/4th of a **Circle**, with a **Circular Arc** used only for meshing, and a **Point** at the location of the middle thermocouple.

GEOMETRY 1

Circle 1 (c1)

1 In the **Geometry** toolbar, click **Circle**.

2 In the **Settings** window for **Circle**, locate the **Size and Shape** section.

3 In the **Radius** text field, type `r_sample`.

4 In the **Sector angle** text field, type `90`.

Circular Arc 1 (ca1)

1 In the **Geometry** toolbar, click **More Primitives** and choose **Circular Arc**.

2 In the **Settings** window for **Circular Arc**, locate the **Radius** section.

3 In the **Radius** text field, type `r_sample/3`.

4 Click **Build All Objects**.

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

Middle Along

1 In the **Geometry** toolbar, click **Point**.

2 In the **Settings** window for **Point**, type `Middle Along` in the **Label** text field.

3 Locate the **Point** section. In the **r** text field, type `r_sample/2`.

4 Click **Build All Objects**.

Mesh Control Edges 1 (mce1)

1 In the **Geometry** toolbar, click **Virtual Operations** and choose **Mesh Control Edges**.

2 On the object **fin**, select Boundary 7 only.

3 In the **Geometry** toolbar, click **Build All**.

DOMAIN ODES AND DAES (DODE)

In the **Domain ODEs and DAEs** interface, the solid species reaction rates are added. Using this interface allows choosing the unit for the dependent variables, namely the densities.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Domain ODEs and DAEs (dode)**.

2 In the **Settings** window for **Domain ODEs and DAEs**, locate the **Units** section.

3 Click **Select Dependent Variable Quantity**.

4 In the **Physical Quantity** dialog box, type `density` in the text field.

5 Click **Filter**.

6 In the tree, select **General>Density (kg/m^3)**.

7 Click **OK**.

8 In the **Settings** window for **Domain ODEs and DAEs**, locate the **Units** section.

9 In the **Source term quantity** table, enter the following settings:

Source term quantity	Unit
Custom unit	kg/(m^3*s)

10 Click to expand the **Dependent Variables** section. In the **Field name (kg/m³)** text field, type `rho`.

11 In the **Number of dependent variables** text field, type `3`.

12 In the **Dependent variables (kg/m³)** table, enter the following settings:

rho_w
rho_is
rho_c

Distributed ODE 1

In the **Source Term** fields, add the decomposition rate expressions for the solid species.

1 In the **Model Builder** window, under **Component 1 (comp1)> Domain ODEs and DAEs (dode)** click **Distributed ODE 1**.

2 In the **Settings** window for **Distributed ODE**, locate the **Source Term** section.

3 In the *f* text-field array, type `-(k_t + k_g + k_is)*rho_w` on the first row.

4 In the *f* text-field array, type `k_is*rho_w - k_c*rho_is` on the second row.

5 In the *f* text-field array, type `k_c * rho_is  + k_c2 * tcs.rho * w_t` on the third row. The dependent variable `w_t` is not yet defined. It will be added in the **Transport of Concentrated Species in Porous Media** Interface.

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 rho_w text field, type `rho_w_init`.

TRANSPORT OF CONCENTRATED SPECIES IN POROUS MEDIA (TCS)

Continue by setting up the mass transfer equations and reactions. The workflow is to first go through the settings for the default features, and then add the features that are needed.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Concentrated Species in Porous Media (tcs)**.

2 In the **Settings** window for **Transport of Concentrated Species in Porous Media**, locate the **Transport Mechanisms** section.

3 From the **Diffusion model** list, choose **Fick's law**.

4 Click to expand the **Dependent Variables** section. In the **Number of species** text field, type `3`.

5 In the **Mass fractions (1)** table, enter the following settings:

w_t
w_g
w_N2

6 Locate the **Species** section. From the **From mass constraint** list, choose **w_N2**.

Species Molar Masses 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Concentrated Species in Porous Media (tcs)** click **Species Molar Masses 1**.

2 In the **Settings** window for **Species Molar Masses**, locate the **Molar Mass** section.

3 In the M_{wt} text field, type `Mw_t`.

4 In the M_{wg} text field, type `Mw_g`.

5 In the M_{wN2} text field, type `Mw_N2`. The parameters for the molar masses were loaded from file and can be found in the **Sample Properties** node under **Global Definitions**.

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Transport of Concentrated Species in Porous Media (tcs)>Porous Medium 1** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Convection** section.

3 From the $\mathbf{u}$ list, choose **Total Darcy velocity field (dl/porous1)**.

Porous Matrix 1

1 In the **Model Builder** window, click **Porous Matrix 1**.

2 In the **Settings** window for **Porous Matrix**, locate the **Matrix Properties** section.

3 In the ε_p text field, type `epsilon`. This parameter was also loaded from file.

Initial Values 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Transport of Concentrated Species in Porous Media (tcs)** click **Initial Values 1**.

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

3 In the $\omega_{0,\mathrm{wt}}$ text field, type `0`.

4 In the $\omega_{0,\mathrm{wg}}$ text field, type `0`.

Since the geometry we want to model is actually a sphere, add a **Symmetry** boundary condition.

Symmetry 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Symmetry**.

2 Select Boundaries 2 and 3 only.

Finally, define the reactions. Add two **Reaction Sources** features; one with the reactions that involve mass transfer to other phases, and one with only gas phase species.

Reaction Sources with Phase Transfer

1 In the **Physics** toolbar, click **Domains** and choose **Reaction Sources**.

2 In the **Settings** window for **Reaction Sources**, type `Reaction Sources with Phase Transfer` in the **Label** text field.

3 Select Domain 1 only.

4 Locate the **Reactions** section. Select the **Mass transfer to other phases** check box.

5 In the R_{wt} text field, type `k_t * rho_w - k_c2 *  w_t * tcs.rho`.

6 In the R_{wg} text field, type `k_g*rho_w`.

Reaction Sources Gas to Gas

1 In the **Physics** toolbar, click **Domains** and choose **Reaction Sources**.

2 In the **Settings** window for **Reaction Sources**, type `Reaction Sources Gas to Gas` in the **Label** text field.

3 Select Domain 1 only.

4 Locate the **Reactions** section. In the R_{wt} text field, type `- k_g2* w_t * tcs.rho`.

5 In the R_{wg} text field, type `k_g2 * w_t * tcs.rho`.

DARCY'S LAW (DL)

Now, define the fluid flow in the system.

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Darcy's Law (dl)> Porous Medium 1** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Fluid Properties** section.

3 From the ρ list, choose **Density (tcs/porous1/fluid1)**.

4 From the μ list, choose **User defined**. In the associated text field, type `viscosity`.

Porous Matrix 1

1 In the **Model Builder** window, 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 `epsilon`.

4 From the κ list, choose **User defined**. From the list, choose **Diagonal**.

5 In the κ table, enter the following settings:

kappa_eff_along	0
0	kappa_eff_across

Initial Values 1

Now we have gone through the settings for the default features. It remains to add a **Mass Source** feature, a **Pressure** boundary condition feature for the external surface, and a **Symmetry** feature.

Mass Source 1

1 In the **Physics** toolbar, click **Domains** and choose **Mass Source**.

2 Select Domain 1 only.

3 In the **Settings** window for **Mass Source**, locate the **Mass Source** section.

4 Click the **Model** button. From the menu, choose **Component 1 (comp1)> Transport of Concentrated Species in Porous Media>tcs.Qmass - Net mass source - kg/(m³·s)**.

5 In the Q_m text field, type `tcs.Qmass`.

Pressure 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Pressure**.

2 Select Boundary 4 only.

Symmetry 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Symmetry**.

2 Select Boundaries 2 and 3 only.

HEAT TRANSFER IN POROUS MEDIA (HT)

The last physics interface to set up is the heat transfer interface. Use the same workflow: go through the default features and then add the additional features that you need. In this case we will add the features **Symmetry**, **Heat Flux**, and **Heat Source**.

Fluid 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Heat Transfer in Porous Media (ht)>Porous Medium 1** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Heat Convection** section.

3 From the $\mathbf{u}$ list, choose **Total Darcy velocity field (dl/porous1)**.

4 Locate the **Model Input** section. From the p_A list, choose **Absolute pressure (dl)**.

5 Locate the **Heat Conduction, Fluid** section. From the k_f list, choose **User defined**. In the associated text field, type `k_f`.

6 Locate the **Thermodynamics, Fluid** section. From the ρ_f list, choose **Density (tcs/porous1/fluid1)**.

7 From the $C_{p,f}$ list, choose **User defined**. In the associated text field, type `cp_f`.

Porous Matrix 1

1 In the **Model Builder** window, 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 `epsilon`.

4 Locate the **Heat Conduction, Porous Matrix** section. From the k_b list, choose **User defined**. From the list, choose **Diagonal**.

5 In the k_b table, enter the following settings:

`k_eff_along`	`0`
`0`	`k_eff_across`

6 Locate the **Thermodynamics, Porous Matrix** section. From the ρ_b list, choose **User defined**. In the associated text field, type `rho_b`.

7 From the $C_{p,b}$ list, choose **User defined**. In the associated text field, type `cp_b`.

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 `T0`.

Symmetry 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Symmetry**.

2 Select Boundaries 2 and 3 only.

Heat Flux 1

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

2 Select Boundary 4 only.

3 In the **Settings** window for **Heat Flux**, locate the **Heat Flux** section.

4 In the q_0 text field, type `q0`.

Heat Source 1

1 In the **Physics** toolbar, click **Domains** and choose **Heat Source**.

2 Select Domain 1 only.

3 In the **Settings** window for **Heat Source**, locate the **Heat Source** section.

4 In the Q_0 text field, type `Q`.

Before we can compute the study, we need to define the mesh that discretizes the modeling domain into finite elements.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.

3 From the list, choose **User-controlled mesh**.

Size

1 In the **Model Builder** window, under **Component 1 (comp1)>Mesh 1** click **Size**.

2 In the **Settings** window for **Size**, locate the **Element Size** section.

3 From the **Predefined** list, choose **Finer**.

Mapped 1

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

2 Drag and drop below **Size**.

3 In the **Settings** window for **Mapped**, locate the **Domain Selection** section.

4 From the **Geometric entity level** list, choose **Domain**.

5 Select Domain 2 only.

Distribution 1

1 Right-click **Mapped 1** and choose **Distribution**.

2 Select Boundary 5 only.

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

4 From the **Distribution type** list, choose **Predefined**.

5 In the **Number of elements** text field, type 25.

Distribution 2

1 In the **Model Builder** window, right-click **Mapped 1** and choose **Distribution**.

2 Select Boundary 7 only.

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

4 In the **Number of elements** text field, type 15.

Size 1

1 In the **Model Builder** window, right-click **Free Triangular 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

3 From the **Geometric entity level** list, choose **Point**.

4 Select Point 1 only.

5 Locate the **Element Size** section. From the **Predefined** list, choose **Finer**.

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

STUDY 1 FORWARD MODEL (INITIAL VALUE BASED)

Set up the study for the forward problem. Add the experimental data to compare it to the results from the forward model. We also add a probe to derive Y (the normalized solid mass) at the same time as we compute the study.

1 In the **Model Builder** window, click **Study 1**.

2 In the **Settings** window for **Study**, type `Study 1 Forward Model (Initial Value Based)` in the **Label** text field.

3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1 Forward Model (Initial Value Based)** 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(0,5,600)`.

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** nodeThe choice **Show Default Solver** creates the node **Solver Configurations** where we can edit the solver settings. Since we know the scales for the dependent variables, we will enter them and not use the default values. If a scale is too high (orders higher than the value of the dependent variable), then we will not get an accurate solution for that variable. If instead the scales are too low, the solver will take more time steps than necessary, giving high accuracy but increasing the computation time.

3 In the **Model Builder** window, expand the **Study 1 Forward Model (Initial Value Based)>Solver Configurations>Solution 1 (sol1)>Dependent Variables 1** node, then click **Pressure (comp1.p)**.

4 In the **Settings** window for **Field**, locate the **Scaling** section.

5 From the **Method** list, choose **Manual**.

6 In the **Model Builder** window, under **Study 1 Forward Model (Initial Value Based)>Solver Configurations>Solution 1 (sol1)>Dependent Variables 1** click **Dependent variable rho_c (comp1.rho_c)**.

7 In the **Settings** window for **Field**, locate the **Scaling** section.

8 From the **Method** list, choose **Manual**.

9 In the **Scale** text field, type `rho_w_init`.

10 In the **Model Builder** window, under **Study 1 Forward Model (Initial Value Based)>Solver Configurations>Solution 1 (sol1)>Dependent Variables 1** click **Dependent variable rho_is (comp1.rho_is)**.

11 In the **Settings** window for **Field**, locate the **Scaling** section.

12 From the **Method** list, choose **Manual**.

13 In the **Scale** text field, type `rho_w_init`.

14 In the **Model Builder** window, under **Study 1 Forward Model (Initial Value Based)>Solver Configurations>Solution 1 (sol1)>Dependent Variables 1** click **Dependent variable rho_w (comp1.rho_w)**.

15 In the **Settings** window for **Field**, locate the **Scaling** section.

16 From the **Method** list, choose **Initial value based**.

17 In the **Model Builder** window, under **Study 1 Forward Model (Initial Value Based)>Solver Configurations>Solution 1 (sol1)>Dependent Variables 1** click **Temperature (comp1.T)**.

18 In the **Settings** window for **Field**, locate the **Scaling** section.

19 From the **Method** list, choose **Initial value based**.

20 In the **Model Builder** window, under **Study 1 Forward Model (Initial Value Based)>Solver Configurations>Solution 1 (sol1)>Dependent Variables 1** click **Mass fraction (comp1.w_g)**.

21 In the **Settings** window for **Field**, locate the **Scaling** section.

22 From the **Method** list, choose **Manual**.

23 In the **Scale** text field, type `0.1`.

24 In the **Model Builder** window, under **Study 1 Forward Model (Initial Value Based)>Solver Configurations>Solution 1 (sol1)>Dependent Variables 1** click **Mass fraction (comp1.w_t)**.

25 In the **Settings** window for **Field**, locate the **Scaling** section.

26 From the **Method** list, choose **Manual**.

27 In the **Scale** text field, type `0.1`.

Since we want to compare the forward problem with the experimental data, add the experimental data. We should also add a probe to derive Y (the normalized solid mass) while solving the model.

RESULTS

Experimental Data

1 In the **Model Builder** window, expand the **Results** node.

2 Right-click **Results>Tables** and choose **Node Group**.

3 In the **Settings** window for **Group**, type `Experimental Data` in the **Label** text field.

Experimental data: Y

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 `parameter_estimation_pyrolysis_wood_experimental_data_Y.txt`.

5 In the **Label** text field, type `Experimental data: Y`.

6 Locate the **Column Headers** section. In the table, enter the following settings:

Column	Header
1	`t(s)`
2	`Y`

Experimental data: T_surface

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Experimental data: T_surface` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

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

5 Locate the **Column Headers** section. In the table, enter the following settings:

Column	Header
1	`t(s)`
2	`T(K)`

6 Right-click **Experimental data: T_surface** and choose **Duplicate**.

Experimental data: T_middle

1 In the **Model Builder** window, under **Results>Tables>Experimental Data** click **Experimental data: T_surface 1**.

2 In the **Settings** window for **Table**, type `Experimental data: T_middle` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

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

5 Locate the **Column Headers** section. In the table, enter the following settings:

Column	Header
1	t(s)
2	T(K)

6 Right-click **Experimental data: T_middle** and choose **Duplicate**.

Experimental data: T_center

1 In the **Model Builder** window, under **Results>Tables>Experimental Data** click **Experimental data: T_middle 1**.

2 In the **Settings** window for **Table**, type `Experimental data: T_center` in the **Label** text field.

3 Locate the **Data** section. Click **Import**.

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

5 Locate the **Column Headers** section. In the table, enter the following settings:

Column	Header
1	t(s)
2	T(K)

Plot the experimental data. Follow these instructions to generate Figure 3 in the model documentation.

Experimental Data

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

2 In the **Settings** window for **1D Plot Group**, type `Experimental Data` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **None**.

4 Click to expand the **Title** section. From the **Title type** list, choose **None**.

Normalized Solid Mass

1 Right-click **Experimental Data** 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 **Red**.

5 Find the **Line markers** subsection. From the **Marker** list, choose **Plus sign**.

6 Click to expand the **Legends** section. Select the **Show legends** check box.

7 Find the **Include** subsection. Select the **Label** check box.

8 Clear the **Headers** check box.

9 In the **Label** text field, type `Normalized Solid Mass`.

10 Right-click **Normalized Solid Mass** and choose **Duplicate**.

Surface Temperature

1 In the **Model Builder** window, under **Results>Experimental Data** click **Normalized Solid Mass 1**.

2 In the **Settings** window for **Table Graph**, type `Surface Temperature` in the **Label** text field.

3 Locate the **Data** section. From the **Table** list, choose **Experimental data: T_surface**.

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

5 Find the **Line markers** subsection. From the **Marker** list, choose **Asterisk**.

6 Right-click **Surface Temperature** and choose **Duplicate**.

Middle Temperature

1 In the **Model Builder** window, under **Results>Experimental Data** click **Surface Temperature 1**.

2 In the **Settings** window for **Table Graph**, type `Middle Temperature` in the **Label** text field.

3 Locate the **Data** section. From the **Table** list, choose **Experimental data: T_middle**.

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

5 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

6 Right-click **Middle Temperature** and choose **Duplicate**.

Center Temperature

1 In the **Model Builder** window, under **Results>Experimental Data** click **Middle Temperature 1**.

2 In the **Settings** window for **Table Graph**, type `Center Temperature` in the **Label** text field.

3 Locate the **Data** section. From the **Table** list, choose **Experimental data: T_center**.

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

5 Find the **Line markers** subsection. From the **Marker** list, choose **Point**.

Experimental Data

1 In the **Model Builder** window, click **Experimental Data**.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Select the **Two y-axes** check box.

4 Select the **x-axis label** check box. In the associated text field, type `Time (s)`.

5 Select the **y-axis label** check box. In the associated text field, type `Normalized Solid Mass (-)`.

6 Select the **Secondary y-axis label** check box. In the associated text field, type `Temperature (K)`.

7 In the table, select the **Plot on secondary y-axis** check boxes for **Surface Temperature**, **Middle Temperature**, and **Center Temperature**.

8 Locate the **Legend** section. From the **Position** list, choose **Middle right**.

9 In the **Experimental Data** toolbar, click **Plot**.

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

11 In the **Experimental Data** toolbar, click **Plot**.

Add the probe to derive Y during computations.

DEFINITIONS

Domain Probe Y Forward Problem

1 In the **Definitions** toolbar, click **Probes** and choose **Domain Probe**.

2 In the **Settings** window for **Domain Probe**, type `Domain Probe Y Forward Problem` in the **Label** text field.

3 In the **Variable name** text field, type `domYforward`.

4 Locate the **Expression** section. In the **Expression** text field, type `Y`.

5 Select the **Description** check box.

6 Click to expand the **Table and Window Settings** section. Click **Add Table**.

RESULTS

Domain Probe Y Forward Problem

1 In the **Model Builder** window, under **Results>Tables** click **Table 5**.

2 In the **Settings** window for **Table**, type `Domain Probe Y Forward Problem` in the **Label** text field.

STUDY 1 FORWARD MODEL (INITIAL VALUE BASED)

Now we are ready to compute the forward study.

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

Follow these instructions to generate Figure 4.

RESULTS

Experimental Data

In the **Model Builder** window, under **Results** right-click **Experimental Data** and choose **Duplicate**.

Forward Model and Experimental Data: Y and T_center

1 In the **Model Builder** window, under **Results** click **Experimental Data 1**.

2 In the **Settings** window for **1D Plot Group**, type `Forward Model and Experimental Data: Y and T_center` in the **Label** text field.

3 In the **Model Builder** window, expand the **Forward Model and Experimental Data: Y and T_center** node.

Middle Temperature, Surface Temperature

1 In the **Model Builder** window, under **Results>Forward Model and Experimental Data: Y and T_center**, Ctrl-click to select **Surface Temperature** and **Middle Temperature**.

2 Right-click and choose **Delete**.

Normalized Solid Mass (exp)

1 In the **Model Builder** window, under **Results>Forward Model and Experimental Data: Y and T_center** click **Normalized Solid Mass**.

2 In the **Settings** window for **Table Graph**, type `Normalized Solid Mass (exp)` in the **Label** text field.

3 Right-click **Results>Forward Model and Experimental Data: Y and T_center>Normalized Solid Mass (exp)** and choose **Duplicate**.

Normalized Solid Mass (forward model)

1 In the **Model Builder** window, under **Results>** **Forward Model and Experimental Data: Y and T_center** click **Normalized Solid Mass (exp) 1**.

2 In the **Settings** window for **Table Graph**, type `Normalized Solid Mass (forward model)` in the **Label** text field.

3 Locate the **Data** section. From the **Table** list, choose **Domain Probe Y Forward Problem**.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

5 Find the **Line markers** subsection. From the **Marker** list, choose **None**.

Center Temperature (forward model)

1 In the **Model Builder** window, right-click **Forward Model and Experimental Data: Y and T_center** and choose **Point Graph**.

2 In the **Settings** window for **Point Graph**, type `Center Temperature (forward model)` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1 Forward Model (Initial Value Based)/Solution 1 (sol1)**.

4 Select Point 1 only.

5 Locate the **y-Axis Data** section. In the **Expression** text field, type `T`.

6 Locate the **y-Axis** section. Select the **Plot on secondary y-axis** check box.

7 Click to expand the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

8 Click to expand the **Legends** section. Select the **Show legends** check box.

9 Find the **Include** subsection. Select the **Label** check box.

10 Clear the **Point** check box.

11 Clear the **Solution** check box.

Forward Model and Experimental Data: Y and T_center

1 In the **Model Builder** window, click **Forward Model and Experimental Data: Y and T_center**.

2 In the **Settings** window for **1D Plot Group**, locate the **Legend** section.

3 From the **Layout** list, choose **Outside graph axis area**.

4 From the **Position** list, choose **Bottom**.

5 In the **Number of rows** text field, type `2`.

6 In the **Forward Model and Experimental Data: Y and T_center** toolbar, click **Plot**.

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

8 In the **Forward Model and Experimental Data: Y and T_center** toolbar, click **Plot**.

Follow these instructions to generate Figure 5.

Experimental Data

In the **Model Builder** window, right-click **Experimental Data** and choose **Duplicate**.

Forward Model and Experimental Data: T_surface and T_middle

1 In the **Model Builder** window, under **Results** click **Experimental Data 1**.

2 In the **Settings** window for **1D Plot Group**, type `Forward Model and Experimental Data: T_surface and T_middle` in the **Label** text field.

3 In the **Model Builder** window, expand the **Forward Model and Experimental Data: T_surface and T_middle** node.

Center Temperature, Normalized Solid Mass

1 In the **Model Builder** window, under **Results>Forward Model and Experimental Data: T_surface and T_middle**, Ctrl-click to select **Normalized Solid Mass** and **Center Temperature**.

2 Right-click and choose **Delete**.

Surface Temperature (exp)

1 In the **Model Builder** window, under **Results>Forward Model and Experimental Data: T_surface and T_middle** click **Surface Temperature**.

2 In the **Settings** window for **Table Graph**, type `Surface Temperature (exp)` in the **Label** text field.

Middle Temperature (exp)

1 In the **Model Builder** window, click **Middle Temperature**.

2 In the **Settings** window for **Table Graph**, type `Middle Temperature (exp)` in the **Label** text field.

Surface Temperature (forward model)

1 In the **Model Builder** window, right-click **Forward Model and Experimental Data: T_surface and T_middle** and choose **Point Graph**.

2 Select Point 4 only.

3 In the **Settings** window for **Point Graph**, type `Surface Temperature (forward model)` in the **Label** text field.

4 Locate the **Data** section. From the **Dataset** list, choose **Study 1 Forward Model (Initial Value Based)/Solution 1 (sol1)**.

5 Select Point 4 only.

6 Locate the **y-Axis Data** section. In the **Expression** text field, type `T`.

7 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dashed**.

8 From the **Color** list, choose **Magenta**.

9 Locate the **Legends** section. Select the **Show legends** check box.

10 Find the **Include** subsection. Select the **Label** check box.

11 Clear the **Point** check box.

12 Clear the **Solution** check box.

13 Right-click **Surface Temperature (forward model)** and choose **Duplicate**.

Middle Temperature (forward model)

1 In the **Model Builder** window, under **Results>**
Forward Model and Experimental Data: T_surface and T_middle click
Surface Temperature (forward model) 1.

2 In the **Settings** window for **Point Graph**, type `Middle Temperature (forward model)` in the **Label** text field.

3 Locate the **Selection** section. Click to select the **Activate Selection** toggle button.

4 Select Point 3 only.

5 Locate the **Coloring and Style** section. From the **Color** list, choose **Black**.

Forward Model and Experimental Data: T_surface and T_middle

1 In the **Model Builder** window, click
Forward Model and Experimental Data: T_surface and T_middle.

2 In the **Settings** window for **1D Plot Group**, locate the **Plot Settings** section.

3 Clear the **Two y-axes** check box.

4 In the **y-axis label** text field, type `Temperature (K)`.

5 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

6 From the **Position** list, choose **Bottom**.

7 In the **Number of rows** text field, type `4`.

8 In the **Forward Model and Experimental Data: T_surface and T_middle** toolbar, click **Plot**.

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

10 In the **Forward Model and Experimental Data: T_surface and T_middle** toolbar, click **Plot**.

Before starting the optimization study, verify that the model has conservation of mass. In other words, check that the mass in the system at any time equals the initial mass in the system.

Mass Conservation Check

1. In the **Results** toolbar, click **Evaluation Group**.
2. In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.
3. From the **Transformation type** list, choose **General**.
4. Select the **Keep child nodes** check box.
5. In the **Column header** text field, type `m(t)/m(0) = 1`.
6. In the **Label** text field, type `Mass Conservation Check`.

Gas and Tar Inside Sample

1. Right-click **Mass Conservation Check** and choose **Integration>Surface Integration**.
2. In the **Settings** window for **Surface Integration**, type `Gas and Tar Inside Sample` in the **Label** text field.
3. Select Domain 1 only.
4. Locate the **Expressions** section. Click **Clear Table**.
5. In the table, enter the following settings:

Expression	Unit	Description
`tcs.rho * (w_t+w_g)*epsilon`	kg	Gas + Tar Inside

Gas and Tar Leaving Sample

1. In the **Model Builder** window, right-click **Mass Conservation Check** and choose **Integration>Line Integration**.
2. In the **Settings** window for **Line Integration**, type `Gas and Tar Leaving Sample` in the **Label** text field.
3. Locate the **Expressions** section. Click **Clear Table**.
4. Select Boundary 4 only.
5. In the table, enter the following settings:

Expression	Unit	Description
`tcs.ntflux_w_g+tcs.ntflux_w_t`	kg/s	Gas + Tar Leaving

6. Locate the **Data Series Operation** section. From the **Transformation** list, choose **Integral**.
7. Select the **Cumulative** check box.

Intermediate + Char

1 Right-click **Mass Conservation Check** and choose **Integration>Surface Integration**.

2 Select Domain 1 only.

3 In the **Settings** window for **Surface Integration**, type `Intermediate + Char` in the **Label** text field.

4 Locate the **Expressions** section. Click **Clear Table**.

5 In the table, enter the following settings:

Expression	Unit	Description
`rho_is + rho_c`	`kg`	`IS + Char`

Wood

1 Right-click **Mass Conservation Check** and choose **Integration>Surface Integration**.

2 In the **Settings** window for **Surface Integration**, type `Wood` in the **Label** text field.

3 Locate the **Expressions** section. Click **Clear Table**.

4 Select Domain 1 only.

5 In the table, enter the following settings:

Expression	Unit	Description
`rho_w`	`kg`	`Wood`

Mass Conservation Check

1 In the **Model Builder** window, click **Mass Conservation Check**.

2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.

3 In the **Expression** text field, type `(int1+int2+int3+int4)`.

4 In the **Mass Conservation Check** toolbar, click **Evaluate**.

MASS CONSERVATION CHECK

1 Go to the **Mass Conservation Check** window.

Normalize with the mass of wood at time 0 s.

2 In the **Settings** window for **Evaluation Group**, locate the **Transformation** section.

3 In the **Expression** text field, type `(int1+int2+int3+int4)/0.0026954`.

4 In the **Mass Conservation Check** toolbar, click **Evaluate**.

5 Go to the **Mass Conservation Check** window.

By looking at the values in column 2 in table **Mass Conservation Check**, we see that the mass is conserved with a precision of at least three decimals.

When setting up a parameter estimation study, start by defining the global least-square objectives.

COMPONENT 1 (COMP1)

T_surface

1 In the **Physics** toolbar, click **Optimization** and choose **Parameter Estimation**.
2 In the **Settings** window for **Global Least-Squares Objective**, type `T_surface` in the **Label** text field.
3 Locate the **Experimental Data** section. From the **Data source** list, choose **Result table**.
4 From the **Result table** list, choose **Experimental data: T_surface**.

We need to enter a model expression for the surface temperature. Add a probe feature for this purpose.

DEFINITIONS

Probes for Parameter Estimation

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Node Group**.
2 In the **Settings** window for **Group**, type `Probes for Parameter Estimation` in the **Label** text field.

Point Probe Surface

1 In the **Definitions** toolbar, click **Probes** and choose **Point Probe**.
2 In the **Settings** window for **Point Probe**, type `Point Probe Surface` in the **Label** text field.
3 In the **Variable name** text field, type `T_surface`.
4 Select Point 4 only.
5 Locate the **Expression** section. In the **Expression** text field, type `T`.
6 Select the **Description** check box.
7 Right-click **Point Probe Surface** and choose **Duplicate**.

Point Probe Middle

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions>Probes for Parameter Estimation** click **Point Probe Surface 1 (point2)**.
2 In the **Settings** window for **Point Probe**, type `Point Probe Middle` in the **Label** text field.

3 In the **Variable name** text field, type `T_middle`.

4 Select Point 3 only.

5 Right-click **Point Probe Middle** and choose **Duplicate**.

Point Probe Center

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions> Probes for Parameter Estimation** click **Point Probe Middle 1 (point3)**.

2 In the **Settings** window for **Point Probe**, type `Point Probe Center` in the **Label** text field.

3 In the **Variable name** text field, type `T_center`.

4 Select Point 1 only.

Domain Probe Y

1 In the **Definitions** toolbar, click **Probes** and choose **Domain Probe**.

2 In the **Settings** window for **Domain Probe**, type `Domain Probe Y` in the **Label** text field.

3 In the **Variable name** text field, type `domY`.

4 Locate the **Expression** section. In the **Expression** text field, type `Y`.

5 Select the **Description** check box.

RESULTS

Probes Parameter Estimation

1 In the **Results** toolbar, click **Table**.

2 In the **Settings** window for **Table**, type `Probes Parameter Estimation` in the **Label** text field.

DEFINITIONS

Point Probe Surface (T_surface)

1 In the **Model Builder** window, under **Component 1 (comp1)>Definitions> Probes for Parameter Estimation** click **Point Probe Surface (T_surface)**.

2 In the **Settings** window for **Point Probe**, click to expand the **Table and Window Settings** section.

3 From the **Output table** list, choose **Probes Parameter Estimation**.

Point Probe Middle (T_middle)

1 In the **Model Builder** window, click **Point Probe Middle (T_middle)**.

2 In the **Settings** window for **Point Probe**, locate the **Table and Window Settings** section.

3 From the **Output table** list, choose **Probes Parameter Estimation**.

Point Probe Center (T_center)

1 In the **Model Builder** window, click **Point Probe Center (T_center)**.

2 In the **Settings** window for **Point Probe**, locate the **Table and Window Settings** section.

3 From the **Output table** list, choose **Probes Parameter Estimation**.

Domain Probe Y (domY)

1 In the **Model Builder** window, click **Domain Probe Y (domY)**.

2 In the **Settings** window for **Domain Probe**, locate the **Table and Window Settings** section.

3 From the **Output table** list, choose **Probes Parameter Estimation**.

Disable the probe that was used for the forward problem. If it is not disabled, it will overwrite the data from the forward problem.

Domain Probe Y Forward Problem (domYforward)

In the **Model Builder** window, under **Component 1 (comp1)>Definitions** right-click **Domain Probe Y Forward Problem (domYforward)** and choose **Disable**.

PARAMETER ESTIMATION

T_surface

1 In the **Model Builder** window, under **Component 1 (comp1)>Parameter Estimation** click **T_surface**.

2 In the **Settings** window for **Global Least-Squares Objective**, locate the **Data Column Settings** section.

3 In the **Model expression** text field, type `T_surface`.

4 In the **Variable name** text field, type `T_surface`.

5 Right-click **Component 1 (comp1)>Parameter Estimation>T_surface** and choose **Duplicate**.

T_mid

1 In the **Model Builder** window, under **Component 1 (comp1)>Parameter Estimation** click **T_surface 1**.

2 In the **Settings** window for **Global Least-Squares Objective**, type `T_mid` in the **Label** text field.

3 Locate the **Experimental Data** section. From the **Result table** list, choose **Experimental data: T_middle**.

4 Locate the **Data Column Settings** section. In the **Model expression** text field, type `T_middle`.

5 In the **Variable name** text field, type `T_middle`.

6 Right-click **T_mid** and choose **Duplicate**.

T_center

1 In the **Model Builder** window, under **Component 1 (comp1)>Parameter Estimation** click **T_mid 1**.

2 In the **Settings** window for **Global Least-Squares Objective**, type `T_center` in the **Label** text field.

3 Locate the **Experimental Data** section. From the **Result table** list, choose **Experimental data: T_center**.

4 Locate the **Data Column Settings** section. In the **Model expression** text field, type `T_center`.

5 In the **Variable name** text field, type `T_center`.

6 Right-click **T_center** and choose **Duplicate**.

Y

1 In the **Model Builder** window, under **Component 1 (comp1)>Parameter Estimation** click **T_center 1**.

2 In the **Settings** window for **Global Least-Squares Objective**, type `Y` in the **Label** text field.

3 Locate the **Experimental Data** section. From the **Result table** list, choose **Experimental data: Y**.

4 Locate the **Data Column Settings** section. In the **Model expression** text field, type `domY`.

5 In the **Variable name** text field, type `domY`.

Now add the Parameter Estimation 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 **Add Study** in the window toolbar.

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

STUDY 2 PARAMETER ESTIMATION

1 In the **Model Builder** window, click **Study 2**.
2 In the **Settings** window for **Study**, type `Study 2 Parameter Estimation` in the **Label** text field.
3 Locate the **Study Settings** section. Clear the **Generate default plots** check box.

Parameter Estimation

1 In the **Study** toolbar, click **Optimization** and choose **Parameter Estimation**.
2 In the **Settings** window for **Parameter Estimation**, locate the **Estimated Parameters** section.
3 Click **Add** four times.
4 In the table, enter the following settings:

Parameter name	Initial value	Scale	Lower bound	Upper bound
A_is_opt (Control parameter to be optimized)	0	1	`A_is_opt_lower`	`A_is_opt_upper`
DH_c_opt (Control parameter to be optimized)	0	1	`DH_c_opt_lower`	`DH_c_opt_upper`
DH_t_opt (Control parameter to be optimized)	0	1	`DH_t_opt_lower`	`DH_t_opt_upper`
hconv_opt (Control parameter to be optimized)	0	1	`hconv_opt_lower`	`hconv_opt_upper`

5 Locate the **Parameter Estimation Method** section. From the **Method** list, choose **BOBYQA**.
6 Find the **Solver settings** subsection. From the **Least-squares time/parameter method** list, choose **Use only least-squares data points**.

Edit the scales for the dependent variables in the same way as for the Forward Study.

Solution 2 (sol2)

1 In the **Study** toolbar, click **Show Default Solver**.
2 In the **Model Builder** window, expand the **Solution 2 (sol2)** node.
3 In the **Model Builder** window, expand the **Study 2 Parameter Estimation>Solver Configurations>Solution 2 (sol2)>Dependent Variables 1** node, then click **Pressure (comp1.p)**.

4 In the **Settings** window for **Field**, locate the **Scaling** section.

5 From the **Method** list, choose **Manual**.

6 In the **Model Builder** window, under **Study 2 Parameter Estimation>Solver Configurations>Solution 2 (sol2)>Dependent Variables 1** click **Dependent variable rho_c (comp1.rho_c)**.

7 In the **Settings** window for **Field**, locate the **Scaling** section.

8 From the **Method** list, choose **Manual**.

9 In the **Scale** text field, type `rho_w_init`.

10 In the **Model Builder** window, under **Study 2 Parameter Estimation>Solver Configurations>Solution 2 (sol2)>Dependent Variables 1** click **Dependent variable rho_is (comp1.rho_is)**.

11 In the **Settings** window for **Field**, locate the **Scaling** section.

12 From the **Method** list, choose **Manual**.

13 In the **Scale** text field, type `rho_w_init`.

14 In the **Model Builder** window, under **Study 2 Parameter Estimation>Solver Configurations>Solution 2 (sol2)>Dependent Variables 1** click **Dependent variable rho_w (comp1.rho_w)**.

15 In the **Settings** window for **Field**, locate the **Scaling** section.

16 From the **Method** list, choose **Initial value based**.

17 In the **Model Builder** window, under **Study 2 Parameter Estimation>Solver Configurations>Solution 2 (sol2)>Dependent Variables 1** click **Temperature (comp1.T)**.

18 In the **Settings** window for **Field**, locate the **Scaling** section.

19 From the **Method** list, choose **Initial value based**.

20 In the **Model Builder** window, under **Study 2 Parameter Estimation>Solver Configurations>Solution 2 (sol2)>Dependent Variables 1** click **Mass fraction (comp1.w_g)**.

21 In the **Settings** window for **Field**, locate the **Scaling** section.

22 From the **Method** list, choose **Manual**.

23 In the **Scale** text field, type `0.1`.

24 In the **Model Builder** window, under **Study 2 Parameter Estimation>Solver Configurations>Solution 2 (sol2)>Dependent Variables 1** click **Mass fraction (comp1.w_t)**.

25 In the **Settings** window for **Field**, locate the **Scaling** section.

26 From the **Method** list, choose **Manual**.

27 In the **Scale** text field, type `0.1`.

Prepare a plot that can be used to inspect the optimization progress during solving. We prepare Figure 6 for this purpose.

RESULTS

Forward Model and Experimental Data: T_surface and T_middle

In the **Model Builder** window, under **Results** right-click **Forward Model and Experimental Data: T_surface and T_middle** and choose **Duplicate**.

Optimized, Forward Model, and Experimental Data: T_surface and T_middle

1 In the **Model Builder** window, expand the **Results> Forward Model and Experimental Data: T_surface and T_middle 1** node, then click **Forward Model and Experimental Data: T_surface and T_middle 1**.

2 In the **Settings** window for **1D Plot Group**, type `Optimized, Forward Model, and Experimental Data: T_surface and T_middle` in the **Label** text field.

3 Locate the **Legend** section. In the **Number of rows** text field, type `6`.

Surface Temperature (forward model)

In the **Model Builder** window, right-click **Surface Temperature (forward model)** and choose **Duplicate**.

Surface Temperature (optimized)

1 In the **Model Builder** window, under **Results>Optimized, Forward Model, and Experimental Data: T_surface and T_middle** click **Surface Temperature (forward model) 1**.

2 In the **Settings** window for **Point Graph**, type `Surface Temperature (optimized)` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 Parameter Estimation/ Solution 2 (sol2)**.

4 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

5 In the **Expression** text field, type `t`.

6 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.

Middle Temperature (forward model)

In the **Model Builder** window, right-click **Middle Temperature (forward model)** and choose **Duplicate**.

Middle Temperature (optimized)

1. In the **Model Builder** window, under **Results>Optimized, Forward Model, and Experimental Data: T_surface and T_middle** click **Middle Temperature (forward model) 1**.
2. In the **Settings** window for **Point Graph**, type `Middle Temperature (optimized)` in the **Label** text field.
3. Locate the **Data** section. From the **Dataset** list, choose **Study 2 Parameter Estimation/ Solution 2 (sol2)**.
4. Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.
5. In the **Expression** text field, type `t`.
6. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.

During optimization, a table will be available to inspect the values for the control parameters and objective function for each model evaluation. To also inspect the values for the physical parameters being optimized, add probes.

DEFINITIONS

Global Variable Probe A_is

1. In the **Definitions** toolbar, click  **Probes** and choose **Global Variable Probe**.
2. In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe A_is` in the **Label** text field.
3. Locate the **Expression** section. In the **Expression** text field, type `A_is`.
4. Click to expand the **Table and Window Settings** section. From the **Output table** list, choose **Probes Parameter Estimation**.
5. In the **Variable name** text field, type `A_is_probe`.
6. Right-click **Global Variable Probe A_is** and choose **Duplicate**.

Global Variable Probe DH_c

1. In the **Model Builder** window, under **Component 1 (comp1)>Definitions> Probes for Parameter Estimation** click **Global Variable Probe A_is 1 (var2)**.
2. In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe DH_c` in the **Label** text field.

3. In the **Variable name** text field, type `DH_c_probe`.
4. Locate the **Expression** section. In the **Expression** text field, type `DH_c`.
5. Right-click **Global Variable Probe DH_c** and choose **Duplicate**.

Global Variable Probe DH_t

1. In the **Model Builder** window, under **Component 1 (comp1)>Definitions>Probes for Parameter Estimation** click **Global Variable Probe DH_c 1 (var3)**.
2. In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe DH_t` in the **Label** text field.
3. In the **Variable name** text field, type `DH_t_probe`.
4. Locate the **Expression** section. In the **Expression** text field, type `DH_t`.
5. Right-click **Global Variable Probe DH_t** and choose **Duplicate**.

Global Variable Probe hconv

1. In the **Model Builder** window, under **Component 1 (comp1)>Definitions>Probes for Parameter Estimation** click **Global Variable Probe DH_t 1 (var4)**.
2. In the **Settings** window for **Global Variable Probe**, type `Global Variable Probe hconv` in the **Label** text field.
3. In the **Variable name** text field, type `hconv_probe`.
4. Locate the **Expression** section. In the **Expression** text field, type `hconv`.

STUDY 2 PARAMETER ESTIMATION

Parameter Estimation

1. In the **Model Builder** window, under **Study 2 Parameter Estimation** click **Parameter Estimation**.
2. In the **Settings** window for **Parameter Estimation**, click to expand the **Output While Solving** section.
3. Select the **Plot** check box.
4. From the **Plot group** list, choose **Optimized, Forward Model, and Experimental Data: T_surface and T_middle**.

   Solve the optimization problem. This takes about one hour.
5. In the **Home** toolbar, click **= Compute**.

The optimization has finished. The optimized values for the physical parameters are seen in table **Probes Parameter Estimation**

RESULTS

Global Evaluation 5

In the **Results** toolbar, click 8.5 **Global Evaluation**.

Values for optimized physical parameters

1 In the **Model Builder** window, click **Global Variable Probe A_is**.

2 In the **Settings** window for **Global Evaluation**, locate the **Data** section.

3 From the **Dataset** list, choose **Study 2 Parameter Estimation/Solution 2 (sol2)**.

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

Expression	Unit	Description
A_is	1/s	Frequency factor w -> is (intermediate solid)
DH_t	J/kg	Heat of reaction wood -> tar
DH_c	J/kg	Heat of reaction intermediate solid -> char
hconv	W/(m^2*K)	External convective heat transfer coefficient

5 Locate the **Data** section. From the **Time selection** list, choose **First**.

6 In the **Label** text field, type `Values for optimized physical parameters`.

7 Click ▾ next to **Evaluate**, then choose **New Table**.

Values for Optimized Physical Parameters

1 In the **Model Builder** window, under **Results>Tables** click **Table 9**.

2 In the **Settings** window for **Table**, type `Values for Optimized Physical Parameters` in the **Label** text field.

Optionally, delete the **Global Evaluation**nodes that are not needed.

Global Evaluation 5, Global Variable Probe DH_c, Global Variable Probe DH_t, Global Variable Probe hconv

1 In the **Model Builder** window, under **Results>Derived Values**, Ctrl-click to select **Global Variable Probe DH_c**, **Global Variable Probe DH_t**, **Global Variable Probe hconv**, and **Global Evaluation 5**.

2 Right-click and choose **Delete**.

Set up plots to inspect the results for the optimized model. Follow the steps below to set up Figure 7.

Forward Model and Experimental Data: Y and T_center

In the **Model Builder** window, under **Results** right-click **Forward Model and Experimental Data: Y and T_center** and choose **Duplicate**.

Optimized, Forward Model, and Experimental Data: Y and T_center

1 In the **Model Builder** window, under **Results** click **Forward Model and Experimental Data: Y and T_center 1**.
2 In the **Settings** window for **1D Plot Group**, type `Optimized, Forward Model, and Experimental Data: Y and T_center` in the **Label** text field.
3 Locate the **Legend** section. In the **Number of rows** text field, type `3`.

Normalized Solid Mass (forward model)

1 In the **Model Builder** window, expand the **Optimized, Forward Model, and Experimental Data: Y and T_center** node.
2 Right-click **Normalized Solid Mass (forward model)** and choose **Duplicate**.

Normalized Solid Mass (optimized)

1 In the **Model Builder** window, under **Results>Optimized, Forward Model, and Experimental Data: Y and T_center** click **Normalized Solid Mass (forward model) 1**.
2 In the **Settings** window for **Table Graph**, type `Normalized Solid Mass (optimized)` in the **Label** text field.
3 Locate the **Data** section. From the **Table** list, choose **Probes Parameter Estimation**.
4 From the **Plot columns** list, choose **Manual**.
5 In the **Columns** list, select **Normalized solid mass (1), Domain Probe Y**.
6 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.

Center Temperature (forward model)

In the **Model Builder** window, right-click **Center Temperature (forward model)** and choose **Duplicate**.

Center Temperature (optimized)

1 In the **Model Builder** window, under **Results>Optimized, Forward Model, and Experimental Data: Y and T_center** click **Center Temperature (forward model) 1**.
2 In the **Settings** window for **Point Graph**, type `Center Temperature (optimized)` in the **Label** text field.
3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 Parameter Estimation/ Solution 2 (sol2)**.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Solid**.

5 From the **Color** list, choose **Blue**.

6 In the **Optimized, Forward Model, and Experimental Data: Y and T_center** toolbar, click **Plot**.

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

8 In the **Optimized, Forward Model, and Experimental Data: Y and T_center** toolbar, click **Plot**.

Solid Species

Let us set up a 3D plot to illustrate how the amounts of the three solid species change during the pyrolysis process. When done, we will have set up Figure 8 in the model documentation.

1 In the **Home** toolbar, click **Add Plot Group** and choose **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Solid Species` in the **Label** text field.

3 Locate the **Color Legend** section. From the **Position** list, choose **Right double**.

4 Click to expand the **Plot Array** section. Select the **Enable** check box.

5 From the **Array shape** list, choose **Square**.

6 From the **Array plane** list, choose **xz**.

Mirror 2D 1

Prepare a dataset that illustrates a half sphere.

1 In the **Results** toolbar, click **More Datasets** and choose **Mirror 2D**.

2 In the **Settings** window for **Mirror 2D**, locate the **Axis Data** section.

3 In row **Point 2**, set **R** to `1`.

4 In row **Point 2**, set **Z** to `0`.

5 Click **Plot**.

Half Sphere

1 In the **Results** toolbar, click **More Datasets** and choose **Revolution 2D**.

2 In the **Settings** window for **Revolution 2D**, type `Half Sphere` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Mirror 2D 1**.

4 Click to expand the **Revolution Layers** section. In the **Revolution angle** text field, type `180`.

5 Click **Plot**.

150s Wood

1 In the **Model Builder** window, right-click **Solid Species** and choose **Surface**.
2 In the **Settings** window for **Surface**, type `150s Wood` in the **Label** text field.
3 Locate the **Data** section. From the **Dataset** list, choose **Half Sphere**.
4 From the **Time (s)** list, choose **Interpolation**.
5 In the **Time** text field, type `150`.
6 Locate the **Expression** section. In the **Expression** text field, type `rho_w/rho_w_init`.

   There are many color tables to choose from. There is also the possibility to create your own. Follow these steps to create three new color tables that will simplify the interpretation of the plot.

7 Click the **Show More Options** button in the **Model Builder** toolbar.
8 In the **Show More Options** dialog box, select **Results>Color Tables** in the tree.
9 In the tree, select the check box for the node **Results>Color Tables**.
10 Click **OK**.

Wood

1 In the **Model Builder** window, under **Results** right-click **Color Tables** and choose **Color Table**.
2 In the **Settings** window for **Color Table**, type `Wood` in the **Label** text field.
3 Locate the **Definition** section. In the table, enter the following settings:

Red	Green	Blue	Length
1	0.72	0.075	20
1	1	1	1
1	1	1	5
0.9	0.9	0.9	0.1

Intermediate

1 Right-click **Color Tables** and choose **Color Table**.
2 In the **Settings** window for **Color Table**, type `Intermediate` in the **Label** text field.
3 Locate the **Definition** section. In the table, enter the following settings:

Red	Green	Blue	Length
0.77	0.22	0.20	20
1	1	1	1

Red	Green	Blue	Length
1	1	1	5
0.9	0.9	0.9	0.1

Char

1 Right-click **Color Tables** and choose **Color Table**.

2 In the **Settings** window for **Color Table**, type `Char` in the **Label** text field.

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

Red	Green	Blue	Length
0.3	0.13	0.06	20
1	1	1	1
1	1	1	5
0.9	0.9	0.9	0.1

150s Wood

1 In the **Model Builder** window, under **Results>Solid Species** click **150s Wood**.

2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

3 Click **Change Color Table**.

4 In the **Color Table** dialog box, select **In Model>Wood** in the tree.

5 Click **OK**.

6 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

7 From the **Color table transformation** list, choose **Reverse**.

8 From the **Color table type** list, choose **Discrete**.

9 Right-click **Results>Solid Species>150s Wood** and choose **Duplicate**.

150s Intermediate Solid

1 In the **Model Builder** window, under **Results>Solid Species** click **150s Wood 1**.

2 In the **Settings** window for **Surface**, type `150s Intermediate Solid` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `rho_is/rho_w_init`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **In Model>Intermediate** in the tree.

6 Click **OK**.

7 Right-click **150s Intermediate Solid** and choose **Duplicate**.

150s Char

1 In the **Model Builder** window, under **Results>Solid Species** click **150s Intermediate Solid 1**.

2 In the **Settings** window for **Surface**, type `150s Char` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `rho_c/rho_w_init`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **In Model>Char** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Surface**, click to expand the **Plot Array** section.

8 Select the **Manual indexing** check box.

9 In the **Column index** text field, type `2`.

150s Wood

In the **Model Builder** window, right-click **150s Wood** and choose **Duplicate**.

270s Wood

1 In the **Model Builder** window, under **Results>Solid Species** click **150s Wood 1**.

2 In the **Settings** window for **Surface**, type `270s Wood` in the **Label** text field.

3 Locate the **Data** section. In the **Time** text field, type `270`.

4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **150s Wood**.

5 Locate the **Plot Array** section. Select the **Manual indexing** check box.

6 In the **Row index** text field, type `1`.

150s Intermediate Solid

In the **Model Builder** window, right-click **150s Intermediate Solid** and choose **Duplicate**.

270s Intermediate Solid

1 In the **Model Builder** window, under **Results>Solid Species** click **150s Intermediate Solid 1**.

2 In the **Settings** window for **Surface**, type `270s Intermediate Solid` in the **Label** text field.

3 Locate the **Data** section. In the **Time** text field, type `270`.

4 Locate the **Inherit Style** section. From the **Plot** list, choose **150s Intermediate Solid**.

5 Locate the **Plot Array** section. Select the **Manual indexing** check box.

6 In the **Row index** text field, type `1`.

7 In the **Column index** text field, type `1`.

150s Char

In the **Model Builder** window, right-click **150s Char** and choose **Duplicate**.

270s Char

1 In the **Model Builder** window, under **Results>Solid Species** click **150s Char 1**.
2 In the **Settings** window for **Surface**, type `270s Char` in the **Label** text field.
3 Locate the **Data** section. In the **Time** text field, type `270`.
4 Locate the **Inherit Style** section. From the **Plot** list, choose **150s Char**.
5 Locate the **Plot Array** section. In the **Row index** text field, type `1`.

270s Wood

In the **Model Builder** window, right-click **270s Wood** and choose **Duplicate**.

410 s Wood

1 In the **Model Builder** window, under **Results>Solid Species** click **270s Wood 1**.
2 In the **Settings** window for **Surface**, type `410 s Wood` in the **Label** text field.
3 Locate the **Data** section. In the **Time** text field, type `410`.
4 Locate the **Plot Array** section. In the **Row index** text field, type `2`.

270s Intermediate Solid

In the **Model Builder** window, right-click **270s Intermediate Solid** and choose **Duplicate**.

410 s Intermediate Solid

1 In the **Model Builder** window, under **Results>Solid Species** click **270s Intermediate Solid 1**.
2 In the **Settings** window for **Surface**, type `410 s Intermediate Solid` in the **Label** text field.
3 Locate the **Data** section. In the **Time** text field, type `410`.
4 Locate the **Plot Array** section. In the **Row index** text field, type `2`.

270s Char

In the **Model Builder** window, right-click **270s Char** and choose **Duplicate**.

410 s Char

1 In the **Model Builder** window, under **Results>Solid Species** click **270s Char 1**.
2 In the **Settings** window for **Surface**, type `410 s Char` in the **Label** text field.
3 Locate the **Data** section. In the **Time** text field, type `410`.
4 Locate the **Plot Array** section. In the **Row index** text field, type `2`.

Solid Species

1 In the **Model Builder** window, click **Solid Species**.

2 In the **Settings** window for **3D Plot Group**, click to expand the **Title** section.

3 From the **Title type** list, choose **None**.

Wood

1 Right-click **Solid Species** and choose **Annotation**.

2 In the **Settings** window for **Annotation**, type `Wood` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Half Sphere**.

4 Locate the **Annotation** section. In the **Text** text field, type `$\frac{\rho_{\omega}}{\rho_{\omega,0}}$`.

5 Select the **LaTeX markup** check box.

6 Locate the **Position** section. In the **z** text field, type `-0.02`.

7 Locate the **Coloring and Style** section. Clear the **Show point** check box.

8 From the **Anchor point** list, choose **Center**.

9 Click to expand the **Plot Array** section. Select the **Manual indexing** check box.

10 Right-click **Wood** and choose **Duplicate**.

Intermediate Solid

1 In the **Model Builder** window, under **Results>Solid Species** click **Wood 1**.

2 In the **Settings** window for **Annotation**, type `Intermediate Solid` in the **Label** text field.

3 Locate the **Annotation** section. In the **Text** text field, type `$\frac{\rho_{is}}{\rho_{\omega,0}}$`.

4 Locate the **Plot Array** section. In the **Column index** text field, type `1`.

5 Right-click **Intermediate Solid** and choose **Duplicate**.

Char

1 In the **Model Builder** window, under **Results>Solid Species** click **Intermediate Solid 1**.

2 In the **Settings** window for **Annotation**, type `Char` in the **Label** text field.

3 Locate the **Annotation** section. In the **Text** text field, type `$\frac{\rho_{c}}{\rho_{\omega,0}}$`.

4 Locate the **Plot Array** section. In the **Column index** text field, type `2`.

Wood

In the **Model Builder** window, right-click **Wood** and choose **Duplicate**.

150 s

1 In the **Model Builder** window, under **Results>Solid Species** click **Wood 1**.

2 In the **Settings** window for **Annotation**, type `150 s` in the **Label** text field.

3 Locate the **Annotation** section. In the **Text** text field, type `150 s`.

4 Locate the **Position** section. In the **z** text field, type `0`.

5 In the **x** text field, type `-0.025`.

6 Right-click **150 s** and choose **Duplicate**.

270 s

1 In the **Model Builder** window, under **Results>Solid Species** click **150 s 1**.

2 In the **Settings** window for **Annotation**, type `270 s` in the **Label** text field.

3 Locate the **Annotation** section. In the **Text** text field, type `270 s`.

4 Locate the **Plot Array** section. In the **Row index** text field, type `1`.

5 Right-click **270 s** and choose **Duplicate**.

410 s

1 In the **Model Builder** window, under **Results>Solid Species** click **270 s 1**.

2 In the **Settings** window for **Annotation**, type `410 s` in the **Label** text field.

3 Locate the **Annotation** section. In the **Text** text field, type `410 s`.

4 Locate the **Plot Array** section. In the **Row index** text field, type `2`.

T, Qmass and Q at 150 s

We have now illustrated the progress of the solid reactions. Now, let us look at the temperature, mass source and heat source. Follow the steps below to set up Figure 9-Figure 11 in the model documentation.

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

2 In the **Settings** window for **2D Plot Group**, type `T, Qmass and Q at 150 s` in the **Label** text field.

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 Parameter Estimation/Solution 2 (sol2)**.

4 From the **Time (s)** list, choose **Interpolation**.

5 In the **Time** text field, type `150`.

6 Click to expand the **Title** section. From the **Title type** list, choose **None**.

7 Locate the **Color Legend** section. Select the **Show units** check box.

8 From the **Position** list, choose **Right double**.

9 Click to expand the **Plot Array** section. Select the **Enable** check box.

10 From the **Array shape** list, choose **Square**.

11 From the **Order** list, choose **Column-major**.

Temperature

1 Right-click **T, Qmass and Q at 150 s** and choose **Annotation**.

2 In the **Settings** window for **Annotation**, type `Temperature` in the **Label** text field.

3 Locate the **Annotation** section. In the **Text** text field, type `$T$`.

4 Select the **LaTeX markup** check box.

5 Locate the **Coloring and Style** section. Clear the **Show point** check box.

6 From the **Anchor point** list, choose **Center**.

7 Click to expand the **Plot Array** section. Select the **Manual indexing** check box.

8 Locate the **Position** section. In the **R** text field, type `0.005`.

9 In the **Z** text field, type `0.0135`.

10 Right-click **Temperature** and choose **Duplicate**.

Mass Source

1 In the **Model Builder** window, under **Results>T, Qmass and Q at 150 s** click **Temperature 1**.

2 In the **Settings** window for **Annotation**, type `Mass Source` in the **Label** text field.

3 Locate the **Annotation** section. In the **Text** text field, type `$Q_{mass}$`.

4 Locate the **Plot Array** section. In the **Row index** text field, type `1`.

5 Right-click **Mass Source** and choose **Duplicate**.

Heat Source

1 In the **Model Builder** window, under **Results>T, Qmass and Q at 150 s** click **Mass Source 1**.

2 In the **Settings** window for **Annotation**, type `Heat Source` in the **Label** text field.

3 Locate the **Annotation** section. In the **Text** text field, type `$Q$`.

4 Locate the **Plot Array** section. In the **Row index** text field, type `2`.

T

1 In the **Model Builder** window, right-click **T, Qmass and Q at 150 s** and choose **Surface**.

2 In the **Settings** window for **Surface**, type `T` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `T`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Thermal>HeatCamera** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

8 From the **Color table type** list, choose **Discrete**.

9 Click to expand the **Plot Array** section. Select the **Manual indexing** check box.

10 Right-click **T** and choose **Duplicate**.

dl.Qm

1 In the **Model Builder** window, under **Results>T, Qmass and Q at 150 s** click **T 1**.

2 In the **Settings** window for **Surface**, type `dl.Qm` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `dl.Qm`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Linear>Viridis** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Surface**, locate the **Plot Array** section.

8 In the **Row index** text field, type `1`.

9 Right-click **dl.Qm** and choose **Duplicate**.

Q

1 In the **Model Builder** window, under **Results>T, Qmass and Q at 150 s** click **dl.Qm 1**.

2 In the **Settings** window for **Surface**, type `Q` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `Q`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Thermal>ThermalWave** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Surface**, locate the **Plot Array** section.

8 In the **Row index** text field, type `2`.

T, Qmass and Q at 150 s

1 Click the **Show Grid** button in the **Graphics** toolbar.

2 In the **Model Builder** window, click **T, Qmass and Q at 150 s**.

3 In the **T, Qmass and Q at 150 s** toolbar, click **Plot**.

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

5 In the **T, Qmass and Q at 150 s** toolbar, click **Plot**.

6 Right-click **T, Qmass and Q at 150 s** and choose **Duplicate**.

T, Qmass and Q at 270 s

1 In the **Model Builder** window, under **Results** click **T, Qmass and Q at 150 s 1**.
2 In the **Settings** window for **2D Plot Group**, type `T, Qmass and Q at 270 s` in the **Label** text field.
3 Locate the **Data** section. In the **Time** text field, type `270`.
4 In the **T, Qmass and Q at 270 s** toolbar, click **Plot**.
5 Click the **Zoom Extents** button in the **Graphics** toolbar.
6 In the **T, Qmass and Q at 270 s** toolbar, click **Plot**.
7 Right-click **T, Qmass and Q at 270 s** and choose **Duplicate**.

T, Qmass and Q at 433 s

1 In the **Model Builder** window, under **Results** click **T, Qmass and Q at 270 s 1**.
2 In the **Settings** window for **2D Plot Group**, type `T, Qmass and Q at 433 s` in the **Label** text field.
3 Locate the **Data** section. In the **Time** text field, type `433`.
4 Click the **Zoom Extents** button in the **Graphics** toolbar.
5 In the **T, Qmass and Q at 433 s** toolbar, click **Plot**.

Pressure, velocity, porosity, and normalized solid mass at 270 s

Now plot the relative pressure, the total Darcy velocity magnitude, porosity, normalized solid mass, and the total Darcy velocity field. This gives Figure 12 in the model documentation.

1 In the **Home** toolbar, click **Add Plot Group** and choose **2D Plot Group**.
2 In the **Settings** window for **2D Plot Group**, type `Pressure, velocity, porosity, and normalized solid mass at 270 s` in the **Label** text field.
3 Locate the **Data** section. From the **Dataset** list, choose **Study 2 Parameter Estimation/ Solution 2 (sol2)**.
4 From the **Time (s)** list, choose **Interpolation**.
5 In the **Time** text field, type `270`.
6 Locate the **Title** section. From the **Title type** list, choose **None**.
7 Locate the **Color Legend** section. Select the **Show units** check box.
8 From the **Position** list, choose **Right double**.
9 Locate the **Plot Array** section. Select the **Enable** check box.
10 From the **Array shape** list, choose **Square**.

Relative Pressure

1 Right-click **Pressure, velocity, porosity, and normalized solid mass at 270 s** and choose **Annotation**.
2 In the **Settings** window for **Annotation**, type `Relative Pressure` in the **Label** text field.
3 Locate the **Annotation** section. In the **Text** text field, type `$p/p_{ref}$`.
4 Select the **LaTeX markup** check box.
5 Locate the **Position** section. In the **R** text field, type `0.005`.
6 In the **Z** text field, type `0.0135`.
7 Locate the **Coloring and Style** section. Clear the **Show point** check box.
8 From the **Anchor point** list, choose **Center**.
9 Locate the **Plot Array** section. Select the **Manual indexing** check box.
10 Right-click **Relative Pressure** and choose **Duplicate**.

Total Darcy Velocity Magnitude

1 In the **Model Builder** window, under **Results>Pressure, velocity, porosity, and normalized solid mass at 270 s** click **Relative Pressure 1**.
2 In the **Settings** window for **Annotation**, type `Total Darcy Velocity Magnitude` in the **Label** text field.
3 Locate the **Annotation** section. In the **Text** text field, type `$U$`.
4 Locate the **Plot Array** section. In the **Column index** text field, type `1`.
5 Right-click **Total Darcy Velocity Magnitude** and choose **Duplicate**.

Porosity

1 In the **Model Builder** window, under **Results>Pressure, velocity, porosity, and normalized solid mass at 270 s** click **Total Darcy Velocity Magnitude 1**.
2 In the **Settings** window for **Annotation**, type `Porosity` in the **Label** text field.
3 Locate the **Annotation** section. In the **Text** text field, type `$\epsilon$`.
4 Locate the **Plot Array** section. In the **Row index** text field, type `1`.
5 In the **Column index** text field, type `0`.
6 Right-click **Porosity** and choose **Duplicate**.

Normalized Solid Mass

1 In the **Model Builder** window, under **Results>Pressure, velocity, porosity, and normalized solid mass at 270 s** click **Porosity 1**.

2 In the **Settings** window for **Annotation**, type `Normalized Solid Mass` in the **Label** text field.

3 Locate the **Annotation** section. In the **Text** text field, type `$Y$`.

4 Locate the **Plot Array** section. In the **Column index** text field, type `1`.

dl.pA/dl.pref

1 In the **Model Builder** window, right-click **Pressure, velocity, porosity, and normalized solid mass at 270 s** and choose **Surface**.

2 In the **Settings** window for **Surface**, type `dl.pA/dl.pref` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `dl.pA/dl.pref`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Wave>Wave** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.

8 From the **Color table type** list, choose **Discrete**.

9 Locate the **Plot Array** section. Select the **Manual indexing** check box.

10 Right-click **dl.pA/dl.pref** and choose **Duplicate**.

dl.U

1 In the **Model Builder** window, under **Results>Pressure, velocity, porosity, and normalized solid mass at 270 s** click **dl.pA/dl.pref 1**.

2 In the **Settings** window for **Surface**, type `dl.U` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `dl.U`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Traffic>Traffic** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Surface**, locate the **Plot Array** section.

8 In the **Column index** text field, type `1`.

dl.u

1 In the **Model Builder** window, right-click **Pressure, velocity, porosity, and normalized solid mass at 270 s** and choose **Arrow Surface**.

2 In the **Settings** window for **Arrow Surface**, type `dl.u` in the **Label** text field.

3 Locate the **Expression** section. In the **R-component** text field, type `dl.u`.

4 In the **Z-component** text field, type `dl.w`.

5 Locate the **Arrow Positioning** section. Find the **R grid points** subsection. In the **Points** text field, type `10`.

6 Find the **Z grid points** subsection. In the **Points** text field, type `10`.

7 Locate the **Coloring and Style** section. From the **Arrow type** list, choose **Cone**.

8 From the **Arrow length** list, choose **Normalized**.

9 From the **Arrow base** list, choose **Center**.

10 Select the **Scale factor** check box. In the associated text field, type `0.14`.

11 From the **Color** list, choose **White**.

12 Click to expand the **Plot Array** section. Select the **Manual indexing** check box.

13 In the **Column index** text field, type `1`.

dl.pA/dl.pref

In the **Model Builder** window, right-click **dl.pA/dl.pref** and choose **Duplicate**.

epsilon

1 In the **Model Builder** window, under **Results>Pressure, velocity, porosity, and normalized solid mass at 270 s** click **dl.pA/dl.pref 1**.

2 In the **Settings** window for **Surface**, type `epsilon` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `epsilon`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Aurora>JupiterAuroraBorealis** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Surface**, locate the **Plot Array** section.

8 In the **Row index** text field, type `1`.

9 Right-click **epsilon** and choose **Duplicate**.

Y

1 In the **Model Builder** window, under **Results>Pressure, velocity, porosity, and normalized solid mass at 270 s** click **epsilon 1**.

2 In the **Settings** window for **Surface**, type `Y` in the **Label** text field.

3 Locate the **Expression** section. In the **Expression** text field, type `Y`.

4 Locate the **Coloring and Style** section. Click **Change Color Table**.

5 In the **Color Table** dialog box, select **Linear>Cividis** in the tree.

6 Click **OK**.

7 In the **Settings** window for **Surface**, locate the **Plot Array** section.

8 In the **Column index** text field, type 1.

Pressure, velocity, porosity, and normalized solid mass at 270 s

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

2 In the **Model Builder** window, click **Pressure, velocity, porosity, and normalized solid mass at 270 s**.

3 In the **Pressure, velocity, porosity, and normalized solid mass at 270 s** toolbar, click **Plot**.