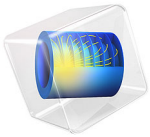

Fermentation in Beer Brewing

Introduction

An important step in brewing beer is the fermentation process. Here, alcohol is formed together with various flavor substances from sugars in the presence of yeast. The initial sugar content, temperature, and yeast type dictate how the fermentation proceeds.

This model consists of two parts. In the first part the fermentation process is efficiently modeled using the Reaction Engineering interface, assuming that the reaction rate is neither mass- nor heat-transfer limited, that is, the system is perfectly mixed.

In the second part of this model, the perfectly mixed model in part 1 is expanded into a sphero-conical tank model accounting for mass transfer, heat transfer and natural convection. In both model setups, it is possible to evaluate several parameters affecting the final alcohol content and taste of the beer. The perfectly mixed example reproduces results in Ref. 1 and Ref. 2.

Model Definition

When brewing beer, the fermentation step is subsequent of malting and mashing, and involves the conversion of sugars to alcohol. The previous steps cover wetting and drying of barley grains to form malt, followed by boiling and mixing the malt, to create a sugary liquid called wort. The fermentation starts as soon as the wort has been cooled down (< 20°C) and yeast has been added to it.

The fermentation usually takes place in a closed tank under anaerobic conditions. The time frame for the fermentation is weeks, but may vary considerably depending on the yeast type and fermentation temperature. The sugar content is mainly made up of three types of sugars: maltose, glucose, and maltotriose. Of these, the maltose content is predominant. Selecting the yeast type is sometimes a bit tricky, but most important is that it should be able to catalyze the fermentation reactions at the chosen process temperature. The type studied in this example thrives at temperatures near 12°C, which is ideal for brewing lager.

REACTION KINETICS

The irreversible reactions taking place during the fermentation process can be written in the following simplified form:

$$G \xrightarrow{x} E + CO_2 + \text{flavors} \quad (1)$$

$$M \xrightarrow{x} E + CO_2 + \text{flavors} \quad (2)$$

$$N \xrightarrow{X} E + CO_2 + \text{flavors} \quad (3)$$

where G, M, and N denote glucose, maltose, and maltotriose, respectively. Furthermore, E stands for ethanol and CO_2 for the carbon dioxide dissolved in the wort. The X notation shows the presence of yeast. Aside from carbon dioxide and ethanol, different flavoring components are formed. This tutorial accounts for two types of flavors: Ethyl acetate (EtAc) and acetaldehyde (AcA). The former, an ester, gives a desirable taste, the latter, an aldehyde, gives a bad tasting beer.

The reaction kinetics are as follows (for reactions 1, 2, and 3). Note that as a consequence of the simplified reaction description, yield coefficients, Y, are used to compute product concentrations:

$$r_i = k_i c_x \quad , \text{i=1,2,3}$$

The fermentation mechanisms depend on the yeast concentration and the reaction rate constant, k_i (SI unit: s^{-1}), can be described using Michaelis–Menten kinetics:

$$k_1 = \frac{k_G c_G}{K_G + c_G}$$

The last two reactions are also inhibited by high sugar concentrations:

$$k_2 = \frac{k_M c_M}{K_M + c_M} \cdot \frac{K'_G}{K'_G + c_G}$$

$$k_3 = \frac{k_N c_N}{K_N + c_N} \cdot \frac{K'_G}{K'_G + c_G} \cdot \frac{K'_M}{K'_M + c_M}$$

k_G, k_M, and k_N are the maximum velocities (SI unit: s^{-1}), K the Michaelis–Menten constant, and K' an inhibition constant for the fermentation reaction. These three properties are temperature dependent as defined by the Arrhenius equation:

$$k_j = A_j e^{\frac{-E}{RT}} \quad , \text{j=G,M,N}$$

$$K_j = A_{Hj} e^{\frac{-E_{Hj}}{RT}}$$

$$K'_j = A'_{Hj} e^{\frac{-E'_{Hj}}{RT}}$$

Here, A is the frequency factor and E is the activation energy.

The yeast concentration is modeled as a free species, with the following reaction rate:

$$R_x = k_x c_x$$

where k_x is the reaction rate constant that depends on the reaction constant of the three governing reactions and the fact that a high yeast concentration inhibits its production:

$$k_x = (Y_{X1}k_1 + Y_{X2}k_2 + Y_{X3}k_3) \cdot \frac{K_X}{K_X + (c_x - c_{x0})^2}$$

where K_X is the yeast growth inhibition constant and c_{x0} the initial yeast concentration in the tank.

The alcohol production needs to be corrected with yield coefficients as well, giving the following total reaction rate:

$$R_E = (Y_{E1}k_1 + Y_{E2}k_2 + Y_{E3}k_3)c_x$$

In similar manner, the production of the ethyl acetate flavor compound can be written as:

$$R_{EtAc} = Y_{EtAc}(k_1 + k_2 + k_3)c_x$$

The acetaldehyde flavor, on the other hand, also decomposes, as given by:

$$R_{AcA} = Y_{AcA}(k_1 + k_2 + k_3)c_x - k_{AcA}c_{AcA}c_x$$

where k_{AcA} is the rate constant for the decomposition of acetaldehyde and is defined with the Arrhenius equation.

Both the gaseous and dissolved carbon dioxide are computed in the example. The reaction rate of the gaseous species is described by:

$$R_{\mathrm{CO2(g)}} = (Y_{C1}k_1 + Y_{C2}k_2 + Y_{C3}k_3)c_x - K_{\mathrm{GL}}(c_{\mathrm{CO2(sat)}} - c_{\mathrm{CO2(l)}})$$

where K_{GL} is the gas to liquid mass transfer coefficient of carbon dioxide and $c_{\mathrm{CO2(sat)}}$ the maximum solubility concentration of carbon dioxide in water.

For the dissolved species, the reaction rate becomes:

$$R_{\mathrm{CO2(l)}} = -K_{\mathrm{GL}}(c_{\mathrm{CO2(sat)}} - c_{\mathrm{CO2(l)}})$$

The reaction data required to simulated the fermentation reactions are tabulated in Table 1.

TABLE 1: REACTION PARAMETERS.

Parameters	Value		Parameters	Value
E_G	$9.46 \cdot 10^4$ J/mol		A'_{HG}	$1.36 \cdot 10^{10}$ mol/m^3
E_M	$4.73 \cdot 10^4$ J/mol		A'_{HM}	$1.42 \cdot 10^{24}$ mol/m^3
E_N	$3.00 \cdot 10^4$ J/mol		A_{AcA}	9.13 m^3/(s·mol)
E_{HG}	$-2.87 \cdot 10^5$ J/mol		Y_{X1}	0.134
E_{HM}	$-6.03 \cdot 10^4$ J/mol		Y_{X2}	0.268
E_{HN}	$-8.33 \cdot 10^4$ J/mol		Y_{X3}	0.402
E'_{HG}	$4.27 \cdot 10^4$ J/mol		Y_{E1}	1.92
E'_{HM}	$1.10 \cdot 10^5$ J/mol		Y_{E2}	3.84
E_{AcA}	$4.64 \cdot 10^4$ J/mol		Y_{E3}	5.76
A_G	$9.51 \cdot 10^{11}$ 1/s		Y_{EtAc}	$9.92 \cdot 10^{-4}$
A_M	$3.68 \cdot 10^3$ 1/s		Y_{AcA}	$1.00 \cdot 10^{-2}$
A_N	$1.10 \cdot 10^1$ 1/s		K_X	$3.65 \cdot 10^5$ mol^2/m^6
A_{HG}	$2.09 \cdot 10^{-53}$ mol/m^3		K_{GL}	$1.94 \cdot 10^{-5}$ 1/s
A_{HM}	$3.40 \cdot 10^{-9}$ mol/m^3		$c_{CO2(sat)}$	$3.90 \cdot 10^2$ mol/m^3
A_{HN}	$2.34 \cdot 10^{-12}$ mol/m^3			

The perfectly mixed model is solved with the Reaction Engineering interface using the Batch, constant volume, reactor type at nonisothermal conditions.

For the three reactions, reactions heats are available: $\Delta H_1 = -91.2$ kJ/mol, $\Delta H_2 = -226.3$ kJ/mol, and $\Delta H_2 = -361.3$ kJ/mol, that are entered into the energy balance settings in the interface. The wort mixture is assumed to have similar thermal properties as water, that is, water is included as solvent. A cooling medium, with a temperature, ΔT_C, lower than the initial tank temperature, cools the fermentation process with the rate, q_v (SI unit: W/(m^3·K)):

$$Q_{ext} = -q_v(T - (T_0 - \Delta T_C))$$

where Q_{ext} is the total heat removed from the reactor (SI unit: W).

Beer fermentation usually takes place in spheroconical tanks (Figure 1). Such a design is suitable for easy separation of yeast from the liquid either at the top or the bottom, and it enables better temperature control. Modern beer brewing equipment often has a built-in cooling jacket, but sometimes the tank is just situated in a cooled environment.

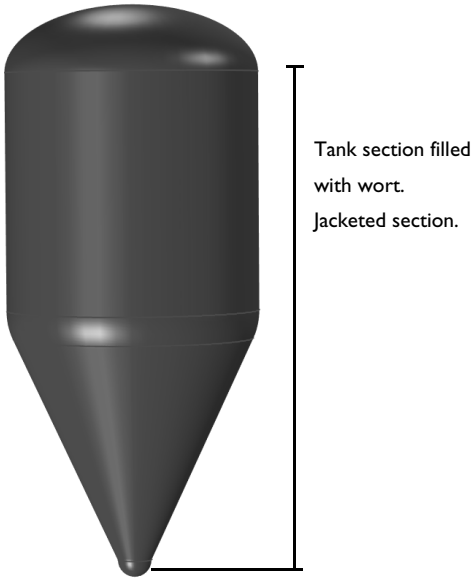

Figure 1: Spheroconical tank for fermentation.

The space-dependent model is created using the Generate Space-Dependent Model feature. The kinetics are thus the same as in the perfectly mixed model. Due to rotational symmetry, you can model the whole system in 2D, using an axisymmetric geometry. The mass transport is modeled using the Transport of Diluted Species interface, the fluid motion with the Laminar Flow interface, and the heat transport using the Heat Transfer in Fluids interface. The wort takes up the part of the reactor as indicated in Figure 1.

The cooling is incorporated as a convective heat flux boundary condition driven by the temperature difference between the tank and the cooling media, as described by:

$$q = h(T_{\text{ext}} - T)$$

where h is an automatically defined heat transfer coefficient for external natural convection.

The only source of mixing is by natural convection, which is achieved by the coupling all three interfaces. As an assumption, the only property affecting the density of the mixture is the temperature. Also, the Boussinesq approximation is used, meaning that in the single-phase flow interface, the density is only varied in the volume force term.

The results from the perfectly mixed model are shown in Figure 2. The temperature in the cooling media and the initial tank temperature are both set to 12°C. The cooling rate is 8 W/(m^3·K).

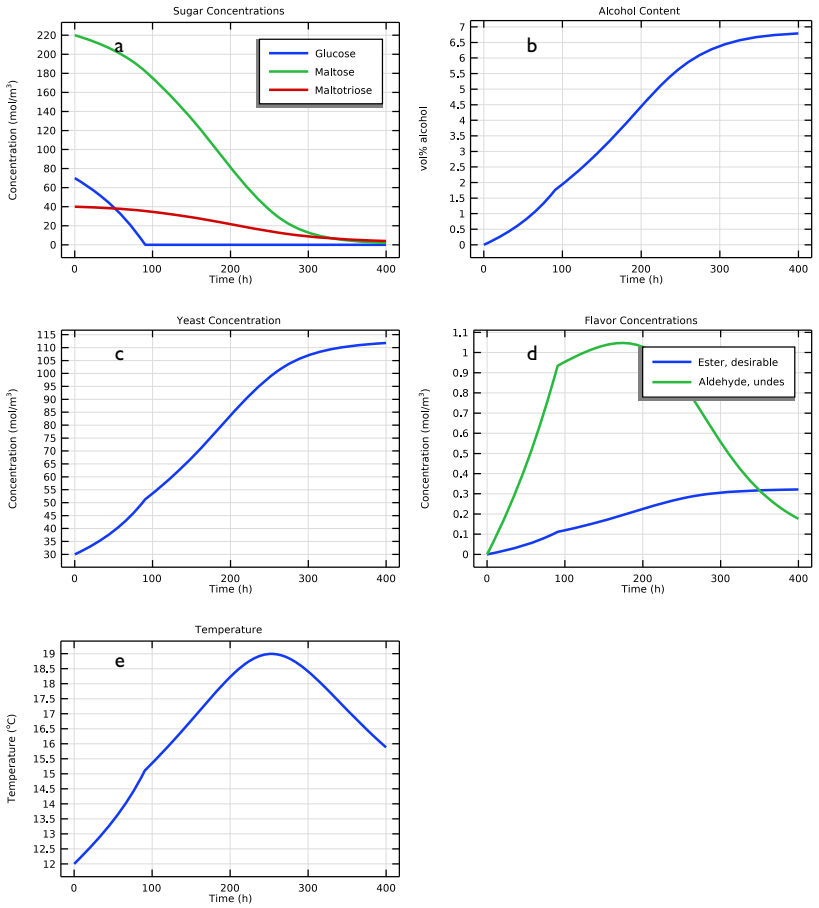

Figure 2: Plots displaying the results of the perfectly mixed model.

At these conditions, all three sugars decrease with time and the alcohol content reaches more than 5 vol%. Unfortunately, this beer will contain a considerable amount of aldehydes and probably taste bad. After reaching a maximum, the aldehyde concentration decreases and it is therefore important to continue the fermentation process long enough to allow the concentration to decrease to acceptable levels. A higher initial yeast

concentration is one approach to decrease the aldehyde content more quickly. The temperature increase observed initially coincides with the quick consumption of glucose. After 60 h, all glucose has been consumed.

The results from the space-dependent model show a very even distribution in concentrations within the tank. In Figure 3, this is illustrated with the concentration of the undesired aldehyde after 3 hours. The same even concentration is seen throughout the whole simulation (24 h)

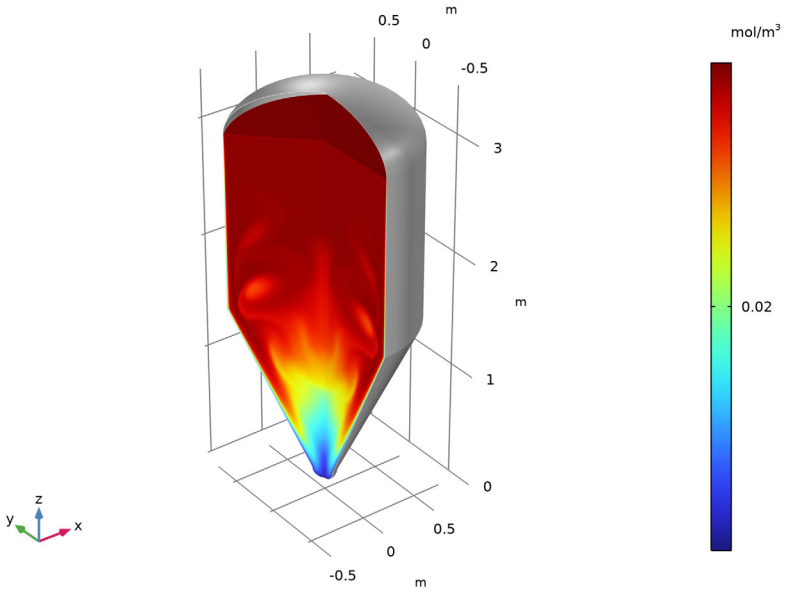

Figure 3: Concentration (mol/m^3) of acetaldehyde after 3 hours.

The well mixed behavior is also seen in Figure 4, showing the velocity magnitude, the temperature difference $T - T_0$, as well as the total energy flux (indicated by arrows), all at 3 h of fermenting. The velocity magnitude illustrates how natural convection creates a downward flow along the cold tank surface. In the temperature plot, the temperature difference is clearly seen along the fluid interface.

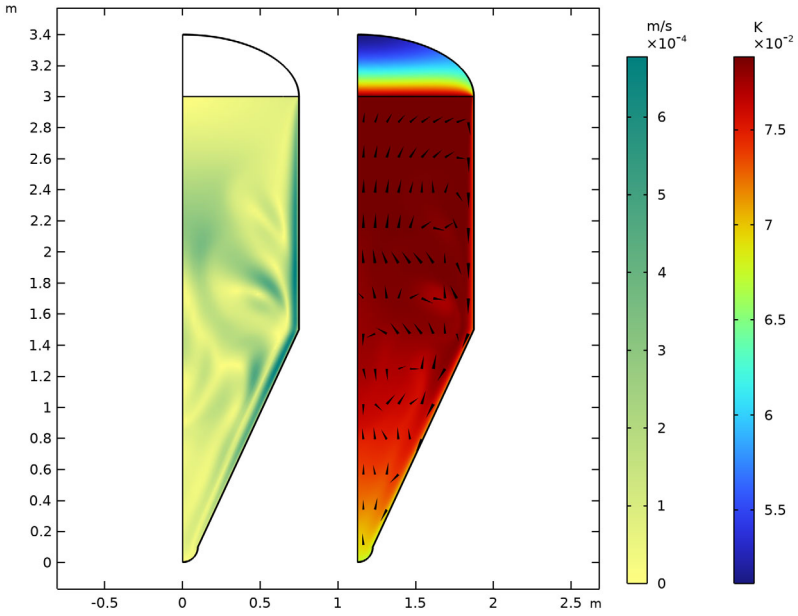

Figure 4: Velocity magnitude, temperature difference $T - T_0$, as well as the total energy flux (indicated by arrows). 3 h of fermentation.

Figure 5 shows the temperature in the top and at the bottom of the tank. During the simulated time frame the temperature is only increased a few degrees from the starting condition. Comparing the temperature reached at 24 h in the 0D model (Figure 2e) with

that in the space-dependent model (Figure 5), we see that the values are practically the same.

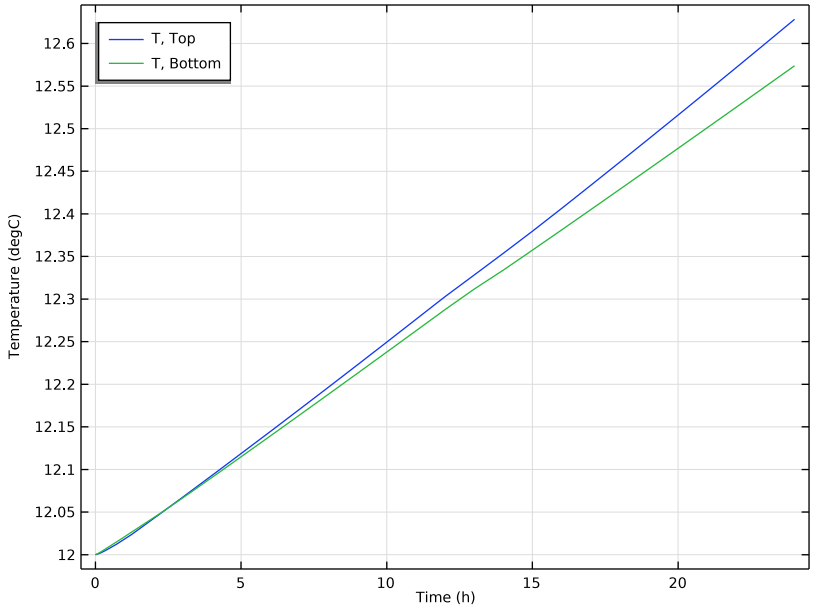

Figure 5: Temperature of the wort as a function of fermentation time. Temperatures at the top and in the bottom of the tank.

References

1. D.A. Gee and W.F. Ramirez, "A Flavour Model for Beer Fermentation," *J. Inst. Brew.*, vol. 100, pp. 321–329, 1994.

2. W.F. Ramirez and J. Maciejowski, "Optimal Beer Fermentation," *J. Inst. Brew.*, vol. 113, no. 3, pp. 325–333, 2007.

Application Library path: `Chemical_Reaction_Engineering_Module/Reactors_with_Mass_and_Heat_Transfer/beer_fermentation`

Modeling Instructions

Setting up 0D (perfectly mixed) model using the **Reaction Engineering** interface.

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

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **0D**.

2 In the **Select Physics** tree, select **Chemical Species Transport>Reaction Engineering (re)**.

3 Click **Add**.

4 Click **Study**.

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

6 Click **Done**.

REACTION ENGINEERING (RE)

Load model parameters and variables from text files.

GLOBAL DEFINITIONS

Parameters 1

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

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

3 Click **Load from File**.

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

DEFINITIONS

Variables 1

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

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

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `beer_fermentation_variables1.txt`.

REACTION ENGINEERING (RE)

Use the **Batch, constant volume**, reactor type (the default) and model nonisothermal conditions by including the **Energy Balance**.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Reaction Engineering (re)**.

2 In the **Settings** window for **Reaction Engineering**, locate the **Energy Balance** section.

3 From the list, choose **Include**.

4 In the Q_{ext} text field, type `-qv*(re.T-(T0-(dTc-273.15[K])))*re.Vr`.

5 Locate the **Mixture Properties** section. From the **Phase** list, choose **Liquid**.

Continue by entering free species, reactions, and a solvent.

Species 1

1 In the **Reaction Engineering** toolbar, click **Species**.

2 In the **Settings** window for **Species**, locate the **Name** section.

3 In the text field, type `X`.

Most reaction products do not fully follow the reaction stoichiometry, therefore enter, where necessary, user defined reaction rates in their respective species nodes.

4 Click to expand the **Reaction Rate** section. From the list, choose **User defined**.

5 In the R_i text field, type `(YXG*kf1+YXM*kf2+YXN*kf3)*re.c_X*KX/(KX+(re.c_X-c0X)^2)`.

Reaction 1

1 In the **Reaction Engineering** toolbar, click **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `G=>E+CO2+EtAc+AcA`.

4 Locate the **Reaction Rate** section. From the list, choose **User defined**.

5 In the r_j text field, type `kf1*re.c_X`.

6 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

7 In the H text field, type `HG`.

Continue to enter user defined reaction rates in the respective species nodes where necessary.

Species: E

1 In the **Model Builder** window, click **Species: E**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 Select the **Enable formula** check box.

4 In the text field, type `C2H5OH`.

5 Locate the **Reaction Rate** section. From the list, choose **User defined**.

6 In the R_i text field, type `(YEG*kf1+YEM*kf2+YEN*kf3)*re.c_X`.

Species: CO2

1 In the **Model Builder** window, click **Species: CO2**.

2 In the **Settings** window for **Species**, locate the **Reaction Rate** section.

3 From the list, choose **User defined**.

4 In the R_i text field, type `max(hCO2*(Csat_CO2-re.c_CO2),0)`.

Species: EtAc

1 In the **Model Builder** window, click **Species: EtAc**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 Select the **Enable formula** check box.

4 In the text field, type `C4H8O2`.

5 Locate the **Reaction Rate** section. From the list, choose **User defined**.

6 In the R_i text field, type `YEtAc*(kf1+kf2+kf3)*re.c_X`.

Species: AcA

1 In the **Model Builder** window, click **Species: AcA**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 Select the **Enable formula** check box.

4 In the text field, type `C2H4O`.

5 Locate the **Reaction Rate** section. From the list, choose **User defined**.

6 In the R_i text field, type `YAcA*(kf1+kf2+kf3)*re.c_X-kAcA*re.c_AcA*re.c_X`.

Reaction 2

1 In the **Reaction Engineering** toolbar, click  **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `M=>E+CO2+EtAc+AcA`.

4 Click **Apply**.

5 Locate the **Reaction Rate** section. From the list, choose **User defined**.

6 In the r_j text field, type `kf2*re.c_X`.

7 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

8 In the H text field, type `HM`.

Reaction 3

1 In the **Reaction Engineering** toolbar, click  **Reaction**.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type `N=>E+CO2+EtAc+AcA`.

4 Click **Apply**.

5 Locate the **Reaction Rate** section. From the list, choose **User defined**.

6 In the r_j text field, type `kf3*re.c_X`.

7 Locate the **Reaction Thermodynamic Properties** section. From the **Enthalpy of reaction** list, choose **User defined**.

8 In the H text field, type `HN`.

Species 1

In the **Reaction Engineering** toolbar, click  **Species**.

Species: N

1 In the **Model Builder** window, click **Species: N**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 Clear the **Enable formula** check box.

Species 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Reaction Engineering (re)** click **Species 1**.

2 In the **Settings** window for **Species**, locate the **Name** section.

3 In the text field, type `H2O`.

4 Locate the **Type** section. From the list, choose **Solvent**.

5 Click to expand the **Thermodynamic Expressions** section. From the list, choose **User defined**.

6 In the C_p text field, type `CpH2O`.

7 In the **Reaction Engineering** toolbar, click  **Species**.

Species 1

1 In the **Settings** window for **Species**, locate the **Name** section.

2 In the text field, type `CO2(g)`.

3 Locate the **Reaction Rate** section. From the list, choose **User defined**.

4 In the R_i text field, type `(YXG*kf1+YXM*kf2+YXN*kf3)*re.c_X-max(hCO2*(Csat_CO2-re.c_CO2),0)`.

Initial Values 1

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

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

3 In the T_0 text field, type `T0`.

4 Locate the **Volumetric Species Initial Values** section. In the table, enter the following settings:

Species	Concentration (mol/m^3)
E	`c0E`
G	`c0G`
H2O	`rhoH2O/re.M_H2O`
M	`c0M`
N	`c0N`
X	`c0X`

Solve the model for 400 h.

STUDY 1

Step 1: Time Dependent

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

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

3 From the **Time unit** list, choose **h**.

4 In the **Output times** text field, type `range(0,1,400)`.

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

6 In the **Relative tolerance** text field, type `1e-6`.

Solution 1 (sol1)

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

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.

3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Absolute Tolerance** section.

4 From the **Tolerance method** list, choose **Manual**.

5 In the **Absolute tolerance** text field, type `1.0E-7`.

6 Click **Compute**.

RESULTS

Sugars

First, create 2a in Figure 2.

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

Global 1

1 In the **Model Builder** window, expand the **Sugars** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Reaction Engineering>re.c_G - Concentration - mol/m³**.

3 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.c_M - Concentration - mol/m³**.

4 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.c_N - Concentration - mol/m³**.

5 Click to expand the **Title** section. From the **Title type** list, choose **Manual**.

6 In the **Title** text area, type `Sugar Concentrations`.

7 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.

8 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.

9 In the table, enter the following settings:

Legends
Glucose
Maltose
Maltotriose

10 In the **Sugars** toolbar, click **Plot**.

Continue with 2b in Figure 2.

Alcohol

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

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

3 Locate the **Plot Settings** section.

4 Select the **y-axis label** check box. In the associated text field, type `vol% alcohol`.

Global 1

1 In the **Model Builder** window, expand the **Alcohol** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions> Variables>Evol - vol% alcohol**.

3 Locate the **Title** section. In the **Title** text area, type `Alcohol Content`.

4 Locate the **Legends** section. Clear the **Show legends** check box.

5 In the **Alcohol** toolbar, click **Plot**.

The yeast concentration plot (2c in Figure 2) is set up following these steps:

Yeast

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

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

3 Locate the **Plot Settings** section. In the **y-axis label** text field, type `Concentration (mol/m<sup>3</sup>)`.

Global 1

1 In the **Model Builder** window, expand the **Yeast** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Reaction Engineering>re.c_X - Concentration - mol/m³**.

3 Locate the **Title** section. In the **Title** text area, type `Yeast Concentration`.

4 In the **Yeast** toolbar, click **Plot**.

The flavors plot (2d) in Figure 2 is set up following these steps:

Flavors

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

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

Global 1

1 In the **Model Builder** window, expand the **Flavors** node, then click **Global 1**.

2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)> Reaction Engineering>re.c_EtAc - Concentration - mol/m³**.

3 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.c_AcA - Concentration - mol/m³**.

4 Locate the **Title** section. In the **Title** text area, type `Flavor Concentrations`.

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

Legends
`Ester, desirable`
`Aldehyde, undesirable`

6 In the **Flavors** toolbar, click **Plot**.

Last, create the temperature plot 2e in Figure 2.

Temperature (re)

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

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

3 Select the **y-axis label** check box. In the associated text field, type `Temperature (<sup>o</sup>C)`.

Global 1

1 In the **Model Builder** window, expand the **Temperature (re)** node, then click **Global 1**.

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

3 In the table, enter the following settings:

Expression	Unit	Description
`re.T-273.15[K]`	K	

4 Locate the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `Temperature`.

6 Locate the **Coloring and Style** section. From the **Width** list, choose **2**.

7 Locate the **Legends** section. Clear the **Show legends** check box.

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

Now, create the space dependent model using the 0D model as a starting point. The Generate Space-Dependent Model feature makes this process straightforward.

REACTION ENGINEERING (RE)

Generate Space-Dependent Model 1

1 In the **Reaction Engineering** toolbar, click **Generate Space-Dependent Model**.

2 In the **Settings** window for **Generate Space-Dependent Model**, locate the **Component Settings** section.

3 From the **Component to use** list, choose **2Daxi: New**.

4 Locate the **Physics Interfaces** section. Find the **Fluid flow** subsection. From the list, choose **Laminar Flow: New**.

5 Find the **Heat transfer** subsection. From the list, choose **Heat Transfer in Fluids: New**.

6 Locate the **Study Type** section. From the **Study type** list, choose **Time dependent**.

7 Locate the **Space-Dependent Model Generation** section. Click **Create/Refresh**.

MULTIPHYSICS

In the **Model Builder** window, expand the **Component 2 (comp2)** node, then click **Multiphysics**.

Nonisothermal Flow 1 (nitf1)

In the **Physics** toolbar, click **Multiphysics Couplings** and choose **Domain> Nonisothermal Flow**.

In the previous step it was seen that the temperature varied in a range of 10 degrees. In this range the density variations are small, and the fluid can be treated as incompressible. To still account for free convection, due to temperature variations, use the Boussinesq approximation.

LAMINAR FLOW 1 (SPF)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Laminar Flow 1 (spf)**.

2 In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.

3 From the **Compressibility** list, choose **Incompressible flow**.

MULTIPHYSICS

Nonisothermal Flow 1 (nitf1)

1 In the **Model Builder** window, under **Component 2 (comp2)>Multiphysics** click **Nonisothermal Flow 1 (nitf1)**.

2 In the **Settings** window for **Nonisothermal Flow**, locate the **Material Properties** section.

3 Select the **Boussinesq approximation** check box.

Reacting Flow, Diluted Species 1 (rfd1)

In the **Physics** toolbar, click  **Multiphysics Couplings** and choose **Domain>Reacting Flow, Diluted Species**.

Import the mesh from a file. The tank geometry is imported together with the mesh.

MESH 1

Import 1

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

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

3 In the **Filename** text field, type `beer_fermentation_mesh.mphbin`.

4 Click  **Import**.

The imported geometry contains a number of selections. These are listed in the **Domain Selections** and **Boundary Selections** sections in the settings window.

Add materials to the geometry.

ADD MATERIAL

1 In the **Home** toolbar, click  **Add Material** to open the **Add Material** window.

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

3 In the tree, select **Built-in>Air**.

4 Click **Add to Component** in the window toolbar.

5 In the tree, select **Built-in>Water, liquid**.

6 Click **Add to Component** in the window toolbar.

MATERIALS

Water, liquid (mat2)

1 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

2 From the **Selection** list, choose **Wort**.

ADD MATERIAL

1 Go to the **Add Material** window.

2 In the tree, select **Built-in>Copper**.

3 Click **Add to Component** in the window toolbar.

4 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Copper (mat3)

1 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.

2 From the **Selection** list, choose **Tank**.

Add variables for the space-dependent model.

DEFINITIONS (COMP2)

Variables 2

1 In the **Model Builder** window, under **Component 2 (comp2)** right-click **Definitions** and choose **Variables**.

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

3 Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `beer_fermentation_variables2.txt`.

Hide all the interior boundaries (used for meshing purposes) except the one that correspond to the vapor liquid interface.

Hide for Physics 1

1 In the **Model Builder** window, right-click **View 1** and choose **Hide for Physics**.

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

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

4 Select Boundaries 6, 8, 16, and 17 only.

CHEMISTRY 1 (CHEM)

In this model, the transport properties used will be those defined from materials. The transport properties computed by the Chemistry interface can thus be disabled.

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Chemistry 1 (chem)**.

2 In the **Settings** window for **Chemistry**, click to expand the **Calculate Transport Properties** section.

3 Clear the **Calculate mixture properties** check box.

The molar masses are automatically computed for species whose names consists of chemical elements from the periodic table. This is also done for species with arbitrary names where the chemical composition has been defined in the **Chemical Formula** section. Add the molar masses for maltose, maltotriose, glucose, and yeast enzymes, for which the composition has not been given.

Species: G

1 In the **Model Builder** window, expand the **Chemistry 1 (chem)** node, then click **Species: G**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 In the M text field, type `MG`.

Species: M

1 In the **Model Builder** window, click **Species: M**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 In the M text field, type `MM`.

Species: N

1 In the **Model Builder** window, click **Species: N**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 In the M text field, type `MN`.

Species: X

1 In the **Model Builder** window, click **Species: X**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 In the M text field, type `MX`.

In the next stage of the modeling process you will set up the physics interfaces describing the mass transport, heat transfer, and fluid flow.

TRANSPORT OF DILUTED SPECIES (TDS)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Transport of Diluted Species (tds)**.

2 In the **Settings** window for **Transport of Diluted Species**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Wort**.

HEAT TRANSFER IN FLUIDS 1 (HT)

1 In the **Model Builder** window, expand the **Transport of Diluted Species (tds)** node, then click **Component 2 (comp2)>Heat Transfer in Fluids 1 (ht)**.

2 In the **Settings** window for **Heat Transfer in Fluids**, locate the **Physical Model** section.

3 In the T_{ref} text field, type `T0`.

Heat Source 1

1 In the **Model Builder** window, under **Component 2 (comp2)>Heat Transfer in Fluids 1 (ht)** click **Heat Source 1**.

2 In the **Settings** window for **Heat Source**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Wort**.

Solid 1

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

2 In the **Settings** window for **Solid**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Tank**.

Fluid 2

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

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

3 From the **Selection** list, choose **Empty tank section**.

4 Locate the **Model Input** section. Click **Make All Model Inputs Editable** in the upper-right corner of the section.

5 From the T list, choose **Temperature (ht)**.

6 From the p_A list, choose **User defined**.

Heat Flux 1

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

2 Select Boundaries 2, 13, 15, 20, and 21 only.

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

4 From the **Flux type** list, choose **Convective heat flux**.

5 From the **Heat transfer coefficient** list, choose **External natural convection**.

6 In the L text field, type `3`.

7 In the T_{ext} text field, type `T0`.

LAMINAR FLOW 1 (SPF)

1 In the **Model Builder** window, under **Component 2 (comp2)** click **Laminar Flow 1 (spf)**.

2 In the **Settings** window for **Laminar Flow**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Wort**.

4 Locate the **Physical Model** section. Select the **Include gravity** check box.

Initial Values 1

1 In the **Model Builder** window, expand the **Laminar Flow 1 (spf)** node, then click **Initial Values 1**.

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

3 In the *p* text field, type `spf.rhoref*g_const*(3-z)`.

Pressure Point Constraint 1

1 In the **Physics** toolbar, click **Points** and choose **Pressure Point Constraint**.

2 Select Point 13 only.

Symmetry 1

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

2 Select Boundaries 10 and 18 only.

STUDY 2

First generate a default solver for fluid and heat transfer only. This produces a default solver setting for natural convection problems, due to the presence of gravity.

Step 1: Time Dependent

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

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

3 From the **Time unit** list, choose **h**.

4 In the **Output times** text field, type `range(0,0.1,4) range(5,1,24)`.

5 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check boxes for **Chemistry 1 (chem)** and **Transport of Diluted Species (tds)**.

Solution 2 (sol2)

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

Now choose to include the mass transport as well.

Step 1: Time Dependent

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

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 In the table, select the **Solve for** check boxes for **Chemistry 1 (chem)** and **Transport of Diluted Species (tds)**.

Solution 2 (sol2)

1 In the **Model Builder** window, expand the **Study 2>Solver Configurations> Solution 2 (sol2)>Dependent Variables 1** node, then click **Concentration (comp2.cAcA)**.

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

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

4 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 1** click **Concentration (comp2.cEtAc)**.

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

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

7 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 1** click **Concentration (comp2.cM)**.

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

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

10 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 1** click **Concentration (comp2.cN)**.

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

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

13 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 1** click **Concentration (comp2.cX)**.

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

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

16 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 1** click **Pressure (comp2.p)**.

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

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

19 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)> Dependent Variables 1** click **Temperature (comp2.T)**.

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

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

Natural convection is present in the wort due to the heat release from the reaction, and the cooling along the tank wall. Restrict the solver from taking too large time steps during the initial phase.

22 In the **Model Builder** window, under **Study 2>Solver Configurations>Solution 2 (sol2)** click **Time-Dependent Solver 1**.

23 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.

24 Select the **Initial step** check box. In the associated text field, type `1/3600`.

25 From the **Maximum step constraint** list, choose **Expression**.

26 In the **Maximum step** text field, type `(60)*(t<4*3600)+(300)*(t>4*3600)`.

Use **Get initial condition** to initialize the datasets and to produce default plot groups. Continue by editing the plot groups before computing the solution.

27 In the **Study** toolbar, click **Get Initial Value**.

Begin by creating the datasets to be used in the plot groups.

RESULTS

Study 2/Wort

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

2 Right-click **Results>Datasets>Study 2/Solution 2 (sol2)** and choose **Duplicate**.

3 In the **Settings** window for **Solution**, type `Study 2/Wort` in the **Label** text field.

Selection

1 In the **Results** toolbar, click **Attributes** and choose **Selection**.

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

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

4 From the **Selection** list, choose **Wort**.

Revolution 2D - Wort

1 In the **Model Builder** window, under **Results>Datasets** right-click **Revolution 2D 1** and choose **Duplicate**.

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

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

Revolution 2D - Wort, Study 2/Wort (sol2)

1 In the **Model Builder** window, under **Results>Datasets**, Ctrl-click to select **Study 2/ Wort (sol2)** and **Revolution 2D - Wort**.

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

Study 2/Tank

In the **Settings** window for **Solution**, type `Study 2/Tank` in the **Label** text field.

Selection

1 In the **Model Builder** window, expand the **Results>Datasets>Study 2/Tank (sol2)** node, then click **Selection**.

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

3 From the **Selection** list, choose **Tank**.

Revolution 2D - Tank

1 In the **Model Builder** window, under **Results>Datasets** click **Revolution 2D - Wort 1**.

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

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

Cut Plane 1

1 In the **Results** toolbar, click  **Cut Plane**.

2 In the **Settings** window for **Cut Plane**, locate the **Data** section.

3 From the **Dataset** list, choose **Revolution 2D - Wort**.

4 Locate the **Plane Data** section. From the **Plane type** list, choose **General**.

5 In row **Point 2**, set **x** to `0`.

6 In row **Point 2**, set **z** to `1`.

7 In row **Point 3**, set **x** to `cos(-90[deg])`.

8 In row **Point 3**, set **y** to `sin(-90[deg])`.

Cut Plane 2

1 Right-click **Cut Plane 1** and choose **Duplicate**.

2 In the **Settings** window for **Cut Plane**, locate the **Plane Data** section.

3 In row **Point 3**, set **x** to `cos(135[deg])`.

4 In row **Point 3**, set **y** to `sin(135[deg])`.

Now edit the plot groups.

Velocity Field and Temperature

1 In the **Model Builder** window, under **Results** click **Concentration, AcA (tds)**.

2 In the **Settings** window for **2D Plot Group**, type `Velocity Field and Temperature` in the **Label** text field.

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

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

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

6 In the **Relative padding** text field, type `0.5`.

7 In the **Velocity Field and Temperature** toolbar, click  **Plot**.

Surface 1

1 In the **Model Builder** window, expand the **Velocity Field and Temperature** node, then click **Surface 1**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `spf.U`.

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

5 From the **Top color** list, choose **Custom**.

6 Click **Define custom colors**.

7 Set the RGB values to 0, 128, and 128, respectively.

8 Click **Add to custom colors**.

9 Click **Show color palette only** or **OK** on the cross-platform desktop.

10 From the **Bottom color** list, choose **Custom**.

11 Click **Define custom colors**.

12 Set the RGB values to 255, 255, and 128, respectively.

13 Click **Add to custom colors**.

14 Click **Show color palette only** or **OK** on the cross-platform desktop.

Surface 2

1 Right-click **Results>Velocity Field and Temperature>Surface 1** and choose **Duplicate**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `T-T0`.

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

Streamline 1

In the **Model Builder** window, under **Results>Velocity Field and Temperature** right-click **Streamline 1** and choose **Delete**.

Arrow Surface 1

1. In the **Model Builder** window, right-click **Velocity Field and Temperature** and choose **Arrow Surface**.
2. In the **Settings** window for **Arrow Surface**, locate the **Expression** section.
3. In the **r-component** text field, type `ht.tefluxr`.
4. In the **z-component** text field, type `ht.tefluxz`.
5. Locate the **Arrow Positioning** section. Find the **r grid points** subsection. In the **Points** text field, type `10`.
6. Locate the **Coloring and Style** section. From the **Arrow type** list, choose **Cone**.
7. From the **Arrow length** list, choose **Logarithmic**.
8. In the **Range quotient** text field, type `1000`.
9. From the **Color** list, choose **Black**.
10. Click to expand the **Plot Array** section. Select the **Manual indexing** check box.
11. In the **Index** text field, type `1`.
12. In the **Velocity Field and Temperature** toolbar, click **Plot**.

Concentration, AcA, 3D (tds)

1. In the **Model Builder** window, expand the **Results>Concentration, AcA, 3D (tds)** node, then click **Concentration, AcA, 3D (tds)**.
2. In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.
3. Clear the **Plot dataset edges** check box.

Surface 2

1. In the **Model Builder** window, under **Results>Concentration, AcA, 3D (tds)** right-click **Surface 1** and choose **Duplicate**.
2. In the **Settings** window for **Surface**, locate the **Data** section.
3. From the **Dataset** list, choose **Revolution 2D - Tank**.
4. Locate the **Expression** section. In the **Expression** text field, type `1`.
5. Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
6. From the **Color** list, choose **Gray**.

Concentration, AcA (Acetaldehyde)

1 In the **Model Builder** window, under **Results** click **Concentration, AcA, 3D (tds)**.

2 In the **Settings** window for **3D Plot Group**, type `Concentration, AcA (Acetaldehyde)` in the **Label** text field.

Temperature, 3D (ht1)

1 In the **Model Builder** window, click **Temperature, 3D (ht1)**.

2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.

3 Clear the **Plot dataset edges** check box.

Surface

1 In the **Model Builder** window, expand the **Temperature, 3D (ht1)** node, then click **Surface**.

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

3 From the **Dataset** list, choose **Revolution 2D - Wort**.

Surface 2

1 Right-click **Surface** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Revolution 2D - Tank**.

4 Locate the **Expression** section. In the **Expression** text field, type `1`.

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

6 From the **Color** list, choose **Gray**.

Arrow Surface 1

1 In the **Model Builder** window, right-click **Temperature, 3D (ht1)** and choose **Arrow Surface**.

2 In the **Settings** window for **Arrow Surface**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Plane 1**.

4 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 2 (comp2)>Heat Transfer in Fluids 1>Domain fluxes>ht.tefluxr, ...,ht.tefluxz - Total energy flux**.

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

6 From the **Color** list, choose **Black**.

Arrow Surface 2

1 Right-click **Arrow Surface 1** and choose **Duplicate**.

2 In the **Settings** window for **Arrow Surface**, locate the **Data** section.

3 From the **Dataset** list, choose **Cut Plane 2**.

Temperature, 3D

1 In the **Model Builder** window, under **Results** click **Temperature, 3D (ht1)**.

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

Delete the default plot groups that are not needed, namely all concentration plots for CO2, E, EtAc, G, M, N and X (in total 16), plus the two Velocity plots. Easiest way to delete them is to Ctrl-click to select all of them and then right-click and choose **Delete**.

Temperature, Top and Bottom

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

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

Point Graph 1

1 Right-click **Temperature, Top and Bottom** and choose **Point Graph**.

2 Select Point 13 only.

Temperature, Top and Bottom

1 In the **Model Builder** window, click **Temperature, Top and Bottom**.

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

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

Point Graph 1

1 In the **Model Builder** window, click **Point Graph 1**.

2 In the **Settings** window for **Point Graph**, locate the **Selection** section.

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

4 Select Point 13 only.

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

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

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

8 Find the **Include** subsection. Select the **Expression** check box.

9 Clear the **Point** check box.

10 Find the **Prefix and suffix** subsection. In the **Suffix** text field, type `, Top`.

Point Graph 2

1 Right-click **Results>Temperature, Top and Bottom>Point Graph 1** and choose **Duplicate**.

2 In the **Settings** window for **Point Graph**, locate the **Selection** section.

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

4 Click **Clear Selection**.

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

6 Select Point 2 only.

7 Locate the **Legends** section. Find the **Prefix and suffix** subsection. In the **Suffix** text field, type `, Bottom`.

8 In the **Temperature, Top and Bottom** toolbar, click **Plot**.

With all the plot groups ready, compute the study and choose the setting to update the plots with results while solving.

STUDY 2

Step 1: Time Dependent

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

2 In the **Settings** window for **Time Dependent**, click to expand the **Results While Solving** section.

3 Select the **Plot** check box.

4 From the **Plot group** list, choose **Velocity Field and Temperature**.

5 From the **Update at** list, choose **Time steps taken by solver**.

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

RESULTS

Velocity Field and Temperature

Time to look at the results.

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

2 From the **Time (h)** list, choose **3**.

3 In the **Velocity Field and Temperature** toolbar, click **Plot**.

Concentration, AcA (Acetaldehyde)

1 In the **Model Builder** window, click **Concentration, AcA (Acetaldehyde)**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Time (h)** list, choose **3**.

4 In the **Concentration, AcA (Acetaldehyde)** toolbar, click **Plot**.

Temperature, 3D

1 In the **Model Builder** window, click **Temperature, 3D**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Time (h)** list, choose **3**.

4 In the **Temperature, 3D** toolbar, click **Plot**.

Surface

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

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

3 From the **Solution parameters** list, choose **From parent**.

Surface 2

1 In the **Model Builder** window, click **Surface 2**.

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

3 From the **Solution parameters** list, choose **From parent**.

Arrow Surface 1

1 In the **Model Builder** window, click **Arrow Surface 1**.

2 In the **Settings** window for **Arrow Surface**, locate the **Data** section.

3 From the **Solution parameters** list, choose **From parent**.

Arrow Surface 2

1 In the **Model Builder** window, click **Arrow Surface 2**.

2 In the **Settings** window for **Arrow Surface**, locate the **Data** section.

3 From the **Solution parameters** list, choose **From parent**.

4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Arrow Surface 1**.

Temperature, Top and Bottom

1 In the **Model Builder** window, under **Results** click **Temperature, Top and Bottom**.

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

3 From the **Position** list, choose **Upper left**.