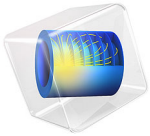

Fermentation in Beer Brewing

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.I

In this example, 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. The 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, which depends on the reaction constant of the three governing reactions and the fact that a high yeast concentration inhibits its production:

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

Here, 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

$$R_{CO_2(g)} = (Y_{C1}k_1 + Y_{C2}k_2 + Y_{C3}k_3)c_x - K_{GL}(c_{co_2(sat)} - c_{co_2(l)})$$

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

For the dissolved species, the reaction rate becomes

$$R_{CO_2(l)} = K_{GL}(c_{co_2(sat)} - c_{co_2(l)})$$

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		$c_{\mathrm{CO2(sat)}}$	$3.90 \cdot 10^{2}$ 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, T_C, cools the fermentation process with the rate, q_v (SI unit: W/(m^3·K)):

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

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

The results from the perfectly mixed model are shown in Figure 1. 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).

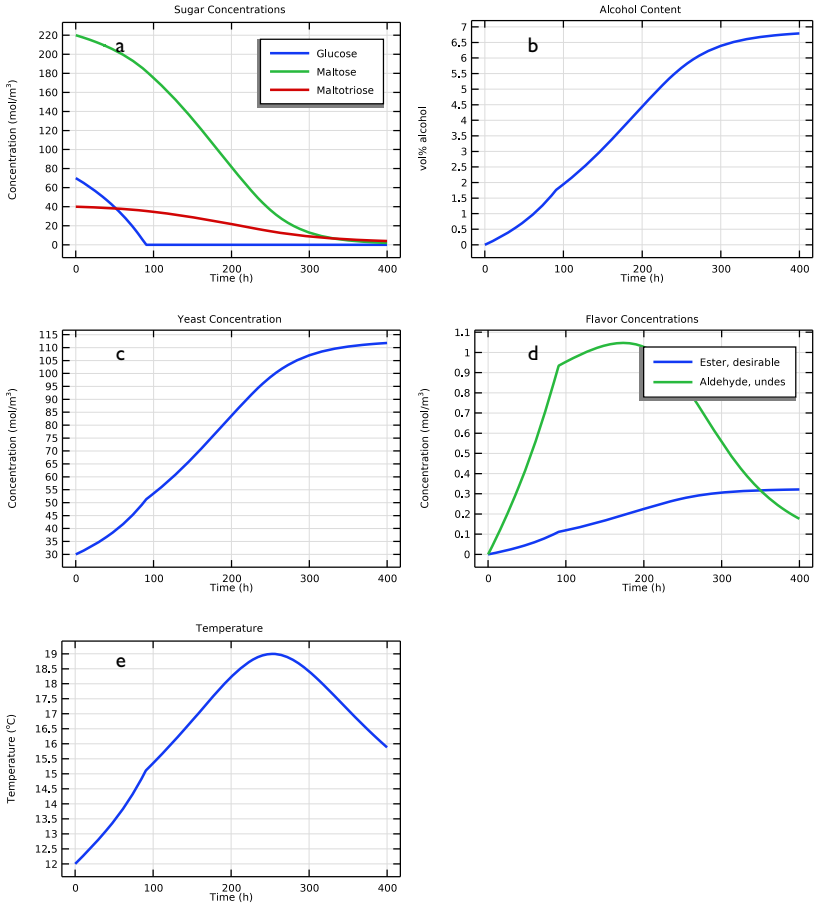

Figure 1: Plots displaying the results of the perfectly mixed model.

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 90 h, all glucose has been consumed.

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 **Energy balance** list, choose **Include**.
4. In the Q_{ext} text field, type `-qv*(re.T-Tc)*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-cOX)^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 `hCO2*(Csat_CO2-re.c_CO2)`.

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**.

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 `max((YXG*kf1+YXM*kf2+YXN*kf3)*re.c_X-hCO2*(Csat_CO2-re.c_CO2),eps)`.

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**.

Notice the warning node that appeared under the **Compile Equations** node in the solver sequence. The warning appeared since there are species in the model without defined heat capacity and molar enthalpy. Modeling nonisothermal conditions requires specifying these thermodynamic properties, usually for each species. In this model though, the properties are not given on a species basis; the heat capacity is defined for the solvent, and the heat of reactions are defined by user defined expressions for each reaction. Therefore, all the required information has been defined, and the warning can be disregarded.

RESULTS

Sugars

First, create 2a in Figure 1.

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 1.

Sugars

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

Alcohol

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

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 - 1**.

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 1) is set up following these steps:

Alcohol

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

Yeast

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

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 1 is set up following these steps:

Sugars

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

Flavors

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

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 1.

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**.