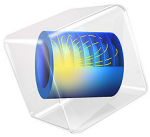

Nonisothermal Plug-Flow Reactor

Introduction

This example considers the thermal cracking of acetone, which is a key step in the production of acetic anhydride. The gas phase reaction takes place under nonisothermal conditions in a plug-flow reactor. As the cracking chemistry is endothermic, control over the temperature in the reactor is essential in order to achieve reasonable conversion. Furthermore, it is illustrated how to affect the conversion of acetone by means of a heat exchanger supplying energy to the system, and how the conversion of acetone is affected by mixing inert into the feed inlet stream.

The example details the use of the predefined Plug flow reactor type in the Reaction Engineering interface of the Chemical Reaction Engineering Module. This model reproduces the results in Ref. 1.

Model Definition

The model simulates the step in the gas-phase production of acetic anhydride where cracking of acetone (A) into ketene (K) and methane (M) occurs:

$$\underset{(A)}{CH_3COCH_3} \longrightarrow \underset{(K)}{CH_2CO} + \underset{(M)}{CH_4}$$

The rate of reaction is:

$$r_1 = k_1 c_A$$

where the rate constant is given by the Arrhenius expression:

$$k_1 = A_1 \exp\left(-\frac{E_1}{R_g T}\right)$$

For the decomposition of acetone described above, the frequency factor is $A_1 = 8.2 \cdot 10^{14}$ (SI unit: 1/s), and the activation energy is $E_1 = 284.5$ (SI unit: kJ/mol). Together with the reacting species nitrogen can also be present as an inert in the system.

The chemical reaction takes place under nonisothermal conditions in a plug-flow reactor, illustrated schematically in Figure 1.

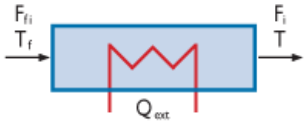

Figure 1: The Plug-flow reactor.

Species mass balances are set up as:

$$\frac{dF_i}{dV} = R_i \tag{1}$$

where F_i is the species molar flow rate (SI unit: mol/s), V is the reactor volume (SI unit: m^3), and R_i is the species rate expression (SI unit: mol/(m^3·s)). Concentrations needed to evaluate rate expressions are described by:

$$c_i = \frac{F_i}{v}$$

where v is the volumetric flow rate (SI unit: m^3/s). By default, the Reaction Engineering interface treats gas phase reacting mixtures as being ideal. Under this assumption the volumetric flow rate is given by:

$$v = \sum_i F_i \frac{R_g T}{p}$$

where p is the pressure (Pa), R_g denotes the ideal gas constant (8.314 J/(mol·K)), and T is the temperature (SI unit: K).

The reactor energy balance is:

$$\sum_i F_i C_{p,i} \frac{dT}{dV} = w_s + Q + Q_{ext} \tag{2}$$

In Equation 2, $C_{p,i}$ represents the species molar heat capacity (SI unit: J/(mol·K)), and w_s is the shaft work per unit volume (SI unit: J/(m^3·s)). Q denotes the heat due to chemical reaction (SI unit: J/(m^3·s)) and is described by:

$$Q = -\sum_j H_j r_j$$

where H_j is the heat produced by reaction j. The term Q_{ext} represents external heat added or removed from the reactor. The present model treats both adiabatic reactor conditions, that is:

$$Q_{\text{ext}} = 0$$

and the situation where the reactor is equipped with a heat exchanger jacket. In the latter case Q_{ext} is given by:

$$Q_{\text{ext}} = Ua(T_{\text{amb}} - T)$$

where U is the overall heat transfer coefficient (SI unit: J/(m^2·s·K)), a is the effective heat transfer area per unit of reactor volume (SI unit: 1/m), and T_{amb} is the temperature of the heat exchanger medium (SI unit: K). The Reaction Engineering interface automatically sets up and solves Equation 1 and Equation 2 as the predefined Plug flow reactor type is selected. As input to the balance equations you need to supply the chemical reaction formula, the Arrhenius parameters, the species thermodynamic properties, as well as the inlet molar feed of reactants.

Working with Thermodynamic Polynomials

The Reaction Engineering interface uses the following set of polynomials as default expressions describing species thermodynamic properties:

$$C_{p,i} = R_g(a_1 + a_2T + a_3T^2 + a_4T^3 + a_5T^4) \tag{3}$$

$$h_i = R_g\left(a_1T + \frac{a_2}{2}T^2 + \frac{a_3}{3}T^3 + \frac{a_4}{4}T^4 + \frac{a_5}{5}T^5 + a_6\right) \tag{4}$$

$$s_i = R_g\left(a_1\ln T + a_2T + \frac{a_3}{2}T^2 + \frac{a_4}{3}T^3 + \frac{a_5}{4}T^4 + a_7\right) \tag{5}$$

Here, $C_{p,i}$ denotes the species' heat capacity (SI unit: J/(mol·K)), T the temperature (K), and R_g the ideal gas constant, 8.314 (J/(mol·K)). Further, h_i is the species' molar enthalpy (SI unit: J/mol), and s_i represents its molar entropy (SI unit: J/(mol·K)). A set of seven coefficients per species are taken as input for the polynomials above. The coefficients a_1 through a_5 relate to the species heat capacity, the coefficient a_6 is associated

with the species enthalpy of formation (at 0 K), and the coefficient a_7 comes from the species entropy of formation (at 0 K).

The format outlined by Equation 3, Equation 4, and Equation 5 is referred to as CHEMKIN or NASA format (Ref. 2). This is a well established format, and database resources list the needed coefficients for different temperature intervals. Many web-based data resources exist for CHEMKIN thermodynamic data and otherwise. For a collection of databases, see Ref. 3. It is therefore often a straightforward task to assemble the thermodynamic data required and then import it into your reaction model.

CREATING A THERMODYNAMIC DATA FILE

CHEMKIN thermodynamic files typically contain blocks of data, one block for each species. Such a data block is illustrated in Figure 2 for gas phase acetone.

```
CH3COCH3_ACETONE  110203H   6C   3O   1    0G   300.000  4000.000 1000.00    0 1
 0.42619220E+01 0.23919538E-01-0.10714477E-04 0.22496890E-08-0.18079303E-12    2
-0.27708340E+05 0.37906279E+01 0.15848079E+01 0.27413605E-01-0.91426603E-05    3
-0.66768869E-09 0.34781512E-12-0.26678575E+05 0.18843809E+02                   4
```

Figure 2: Thermodynamic data block on the CHEMKIN format.

The first line starts with the species label, given with a maximum of 18 characters, followed by a 6 character comment space. Then follows a listing of the type and number of atoms that constitute the species. The `G` comments that this is gas phase data. The line ends with listing of three temperatures, defining two temperature intervals. Lines 2 through 4 contain two sets of the polynomial coefficients, a_1 through a_7. The first set of coefficients is valid for the upper temperature interval, and the second for the lower interval.

A complete CHEMKIN thermodynamics file has the structure illustrated in Figure 3.

```
THERMO
   300.000  2000.000 2000.00
A                 110203H   6C   3O   1    0G   300.000  4000.000 1000.00    0 1
 0.42619220E+01 0.23919538E-01-0.10714477E-04 0.22496890E-08-0.18079303E-12    2
-0.27708340E+05 0.37906279E+01 0.15848079E+01 0.27413605E-01-0.91426603E-05    3
-0.66768869E-09 0.34781512E-12-0.26678575E+05 0.18843809E+02                   4
M                 110203H   4C   1    0    0G   300.000  4000.000 1000.00    0 1
 0.47238333E+00 0.12680758E-01-0.55093741E-05 0.11295575E-08-0.89103779E-13    2
-0.96424500E+04 0.16199090E+02 0.38717898E+01-0.42480466E-02 0.24540181E-04    3
-0.21780766E-07 0.63010622E-11-0.10144425E+05 0.66008135E+00                   4
K                 110203H   2C   2O   1    0G   300.000  4000.000 1000.00    0 1
 0.47307523E+01 0.84849084E-02-0.37289848E-05 0.77166210E-09-0.61322345E-13    2
-0.76492303E+04-0.68485049E+00 0.15410946E+01 0.21513643E-01-0.25750130E-04    3
 0.18486377E-07-0.55939702E-11-0.69557078E+04 0.14808619E+02                   4
N2                110203N   2    0    0    0G   300.000  4000.000 1000.00    0 1
 0.27292633E+01 0.17776002E-02-0.76185598E-06 0.15386678E-09-0.11961307E-13    2
-0.83679340E+03 0.70662127E+01 0.36962069E+01-0.12983164E-02 0.24640713E-05    3
-0.93801238E-09-0.37036420E-13-0.10631030E+04 0.22199845E+01                   4
END
```

Figure 3: Thermodynamic data file on the CHEMKIN format.

The keyword `thermo` always starts the text file. The subsequent line lists three temperatures, defining two temperature intervals. These intervals are used if no intervals are provided in the species specific data. Then follows the species data blocks, in any order. The keyword `end` is the last entry in the file.

The data file reproduced in Figure 3 is used in the present model. It was constructed by creating a text-file with species data blocks from the Sandia National Labs Thermodynamics Resource.

USING SUBSETS OF THERMODYNAMIC COEFFICIENTS

In some instances, not all coefficients a_1 through a_7 are available. Coefficients may also be on a format differing from the NASA or CHEMKIN style. Input parameters can still be put on the form of Equation 3, Equation 4, and Equation 5, as illustrated below.

For species A, K, M, and N2, Ref. 1 lists polynomials for the heat capacity on the form:

$$C_{p,i} = a_1' + a_2' T + a_3' T^2$$

Furthermore, the species enthalpies of formation at $T_{\text{ref}} = 298$ K are provided:

SPECIES	a_1'	a_2'	a_3'	h(298)
A	26.63	0.183	-45.86e-6	-216.67e3
K	20.04	0.0945	-30.95e-6	-61.09e3

SPECIES	a_1'	a_2'	a_3'	h(298)
M	13.39	0.077	-18.71e-6	-71.84e3
N2	6.25	8.78e-3	-2.1e-8	0

The data in the table above can be correlated with the polynomials given by Equation 3 and Equation 4 by noting the relations:

$$a_n = \frac{a_n'}{R_g} \qquad n = 1, \ldots, 5 \tag{6}$$

$$a_6 = \frac{h(T_{ref})}{R_g} - \left(a_1 T_{ref} + \frac{a_2}{2} T_{ref}^2 + \frac{a_3}{3} T_{ref}^3\right) \tag{7}$$

Using Equation 6 and Equation 7, you find the coefficients to enter in the Reaction Engineering interface.

SPECIES	a_1	a_2	a_3	a_6
A	3.20	2.20e-2	-5.52e-6	-2.79e4
K	2.41	1.14e-2	-3.72e-6	-8.54e3
M	1.61	9.26e-3	-2.25e-6	-9.87e3
N2	0.752	1.06e-3	-2.53e-9	-2.71e2

Read more about how to work with thermodynamic data in the section *Transport Properties* in the *Chemical Reaction Engineering Module User's Guide*.

Results and Discussion

A 5 m^3 plug-flow reactor is simulated both for adiabatic conditions and with heat exchange. The reactor is fed with pure acetone at 1035 K. 18.8 mol/m^3 acetone is set to enter with a volumetric flow of 2 m^3/s. Figure 4 shows the reactor temperature as a function of the reactor volume for both cases. In the adiabatic case, with no additional heating, the reactor temperature decreases along the reactor length since the cracking reaction is endothermic. On the other hand, the temperature profile as a heat exchanger supplies energy increases after first passing through a minimum. This is explained by Figure 5 where the reaction rates are shown. The minimum is due to the energy demand of the cracking reaction being dominant initially. However, as the reaction rate drops off,

the heat exchanger starts to heat up the system. The heating rate decreases with the temperature difference between the heat exchanger medium and reacting fluid.

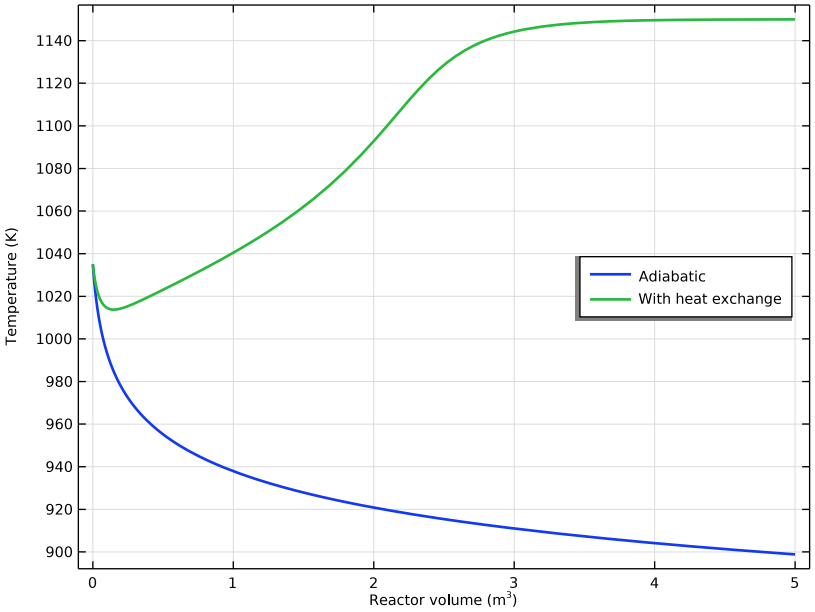

Figure 4: The reactor temperature (K) as a function of reactor volume (m^3) for the two investigated cases.

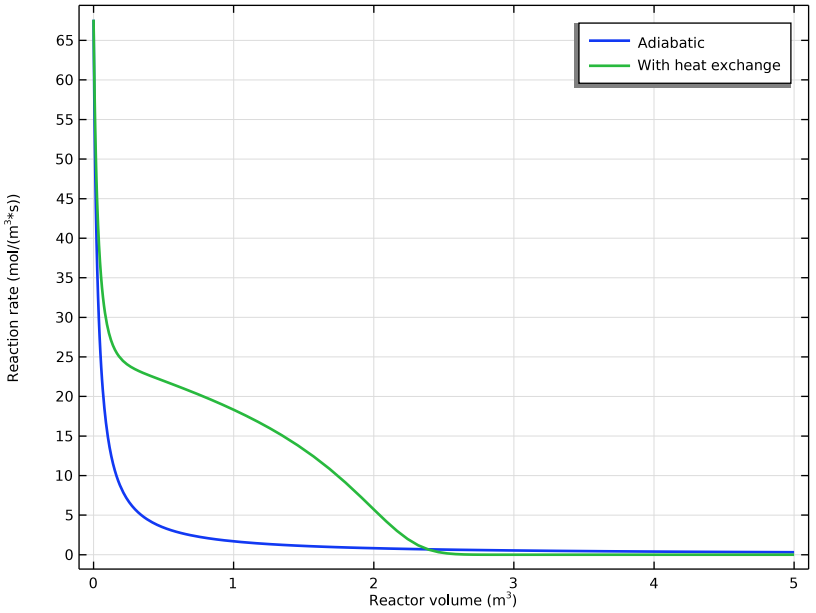

Figure 5: The reaction rates (mol/(m^3·s)) as functions of reactor volume (m^3) for the two investigated cases.

Figure 6 shows the conversion of acetone. The reactor conversion is considerably lower at the reactor outlet in the adiabatic case than with heat exchange.

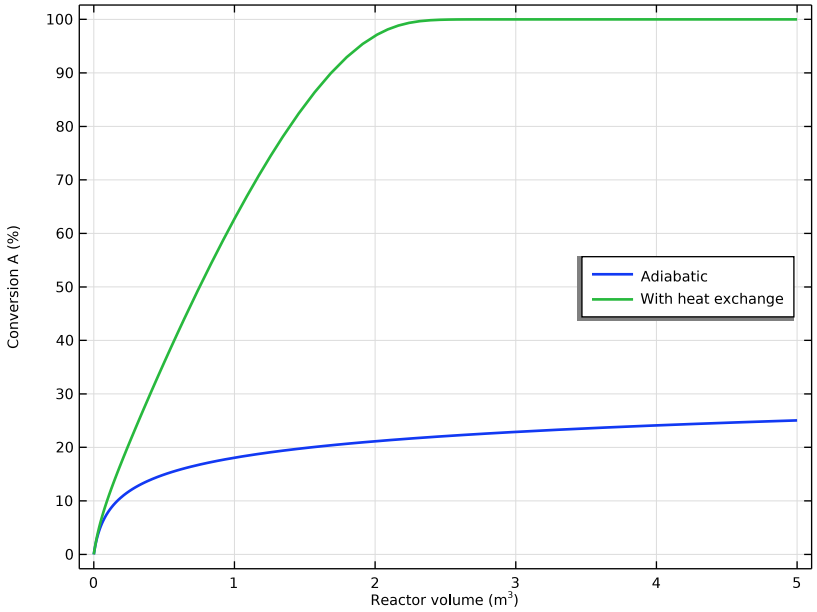

Figure 6: The conversion of acetone (%) as a function of reactor volume (m^3) for the two investigated cases.

If the feed inlet stream contains an additional amount of nitrogen inert the conversion of A becomes more efficient at adiabatic conditions. This is shown for three different molar fractions of acetone in the inlet in Figure 7. The explanation is that the inert acts as a heat supply to the endothermic reaction.

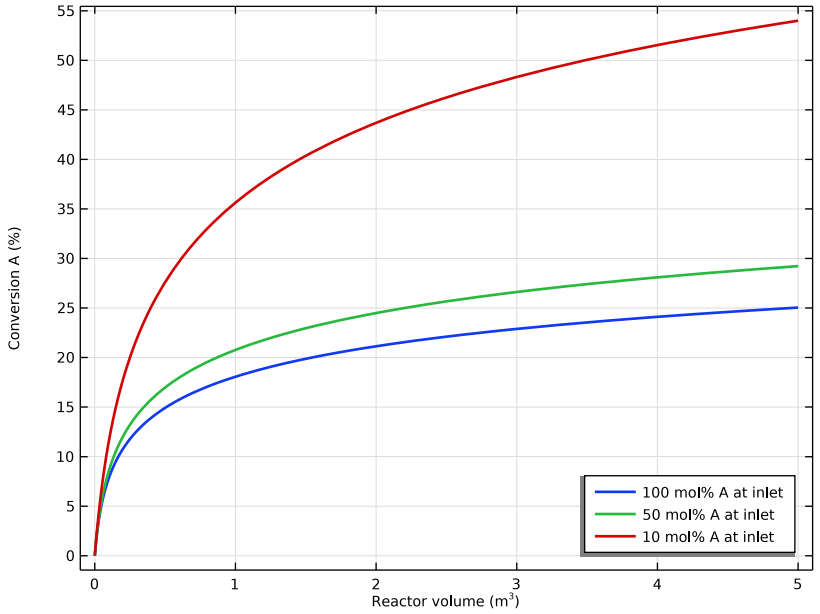

Figure 7: The conversion of acetone (%) as a function of reactor volume (m^3) for 100 mol%, 50 mol%, and 10 mol% of acetone in the feed inlet stream.

References

1. H.S. Fogler, *Elements of Chemical Reaction Engineering*, 3rd ed., Prentice Hall PTR, example 8-7, pp. 462–468, 1999.

2. S. Gordon and B.J. McBride, *Computer Program for Calculation of Complex Chemical Equilibrium Compositions, Rocket Performance, Incident and Reflected Shocks, and Chapman-Jouquet Detonations*, NASA-SP-273, 1971.

3. See, for example https://www.comsol.com/chemical-reaction-engineering-module#specs

Application Library path: `Chemical_Reaction_Engineering_Module/Tutorials/nonisothermal_plug_flow`

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 **Preset Studies for Selected Physics Interfaces> Stationary Plug Flow**.

6 Click **Done**.

GLOBAL DEFINITIONS

Add a set of model parameters by importing their definitions from a data text file provided with the **Application Library**.

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 `nonisothermal_plug_flow_parameters.txt`.

REACTION ENGINEERING (RE)

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

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

3 From the **Reactor type** list, choose **Plug flow**.

4 Locate the **Energy Balance** section. From the list, choose **Include**.

5 Click to expand the **Mixture Properties** section. In the *p* text field, type `P_reactor`.

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 `A=>K+M`.

4 Locate the **Rate Constants** section. Select the **Use Arrhenius expressions** check box.

5 In the A^{f} text field, type `Af_reaction`.

6 In the E^{f} text field, type `Ef_reaction`.

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 `N2`.

Set inlet properties derived from the volumetric flow and concentration of A at the inlet.

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 $T_{0,\mathrm{in}}$ text field, type `T_inlet`.

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

Species	Molar flow rate (mol/s)
A	Finlet_A
N2	Finlet_N2

Import material and thermal properties for the reaction with the **CHEMKIN Import for Species property**.

5 In the **Model Builder** window, click **Reaction Engineering (re)**.

6 In the **Settings** window for **Reaction Engineering**, click to expand the **CHEMKIN Import for Species Properties** section.

7 Click **Browse**.

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

9 Click **Import**.

Also add a variable expression for monitoring the conversion of A. This will be used later on when postprocessing the solution.

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. In the table, enter the following settings:

Name	Expression	Unit	Description
X_A	(re.F0_A-re.F_A)/re.F0_A*100		Conversion, A

Solve first for adiabatic conditions.

STUDY 1

Step 1: Stationary Plug Flow

1. In the **Model Builder** window, under **Study 1** click **Step 1: Stationary Plug Flow**.
2. In the **Settings** window for **Stationary Plug Flow**, locate the **Study Settings** section.
3. In the **Output volumes** text field, type `range(0,0.05,5)`.
4. In the **Home** toolbar, click **Compute**.

Save a copy of the adiabatic solution.

Solution 1 (sol1)

1. In the **Model Builder** window, expand the **Study 1>Solver Configurations** node.
2. Right-click **Solution 1 (sol1)** and choose **Solution>Copy**.

Adiabatic

1. In the **Model Builder** window, under **Study 1>Solver Configurations** click **Solution 1 - Copy 1 (sol2)**.
2. In the **Settings** window for **Solution**, type `Adiabatic` in the **Label** text field.

Add a heat source from a heat exchanger.

REACTION ENGINEERING (RE)

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. In the Q text field, type `Ua*(T_x-re.T)`.

Solve for the heat exchanged plug flow reactor.

STUDY 1

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

Solution 1 (sol1)

In the **Model Builder** window, under **Study 1>Solver Configurations** right-click **Solution 1 (sol1)** and choose **Solution>Copy**.

With heat exchange

1 In the **Model Builder** window, under **Study 1>Solver Configurations** click **Solution 1 - Copy 1 (sol3)**.

2 In the **Settings** window for **Solution**, type `With heat exchange` in the **Label** text field.

Remove the heat exchange and solve for a **Parametric Sweep** of three molar fractions of A, 0 mol%, 50 mol%, and 90 mol%, at the inlet at adiabatic conditions.

REACTION ENGINEERING (RE)

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 In the Q text field, type `0`.

STUDY 1

Parametric Sweep

1 In the **Study** toolbar, click **Parametric Sweep**.

2 In the **Settings** window for **Parametric Sweep**, locate the **Study Settings** section.

3 Click **Add**.

4 In the table, enter the following settings:

Parameter name	Parameter value list	Parameter unit
A_frac (Inlet mole fraction A)	`1 0.5 0.1`	1

5 In the **Study** toolbar, click **Compute**.

Parametric Solutions 1 (sol4)

In the **Model Builder** window, under **Study 1>Solver Configurations** right-click **Parametric Solutions 1 (sol4)** and choose **Solution>Copy**.

With inert

1 In the **Model Builder** window, under **Study 1>Solver Configurations** click **Parametric Solutions 1 - Copy 1 (sol8)**.

2 In the **Settings** window for **Solution**, type `With inert` in the **Label** text field.

Start with Figure 4, where the temperature change is displayed for the adiabatic and heat exchanged cases.

RESULTS

The following instructions generate Figure 4 through Figure 7.

Temperature (re)

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

2 In the **Settings** window for **1D Plot Group**, click to expand the **Title** section.

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

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

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 **Data** section.

3 From the **Dataset** list, choose **Study 1/Adiabatic (sol2)**.

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

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

6 In the table, enter the following settings:

Legends
Adiabatic

Global 2

1 Right-click **Results>Temperature (re)>Global 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Study 1/With heat exchange (sol3)**.

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

Legends
With heat exchange

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

Continue with Figure 5, displaying the reaction rate for the adiabatic and heat exchanged cases.

1D Plot Group 5

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

Reaction rate (re)

1. In the **Model Builder** window, under **Results** click **Molar Flow Rate (re) 1**.
2. In the **Settings** window for **1D Plot Group**, type `Reaction rate (re)` in the **Label** text field.
3. Locate the **Title** section. From the **Title type** list, choose **None**.

Global 2

Right-click **Reaction rate (re)** and choose **Global**.

Global 1

1. In the **Settings** window for **Global**, locate the **Data** section.
2. From the **Dataset** list, choose **Study 1/Adiabatic (sol2)**.
3. Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.r_1 - Reaction rate - mol/(m³·s)**.
4. Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
5. Locate the **Legends** section. From the **Legends** list, choose **Manual**.
6. In the table, enter the following settings:

Legends
Adiabatic

Global 2

1. In the **Model Builder** window, click **Global 2**.
2. In the **Settings** window for **Global**, locate the **Data** section.
3. From the **Dataset** list, choose **Study 1/With heat exchange (sol3)**.
4. Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering>re.r_1 - Reaction rate - mol/(m³·s)**.
5. Locate the **Coloring and Style** section. From the **Width** list, choose **2**.
6. Locate the **Legends** section. From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
With heat exchange

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

Next is Figure 6 illustrating the conversion of acetone for the adiabatic and heat exchanged cases.

Conversion A (re)

1 In the **Model Builder** window, under **Results** click **Molar Flow Rate (re)**.

2 In the **Settings** window for **1D Plot Group**, type `Conversion A (re)` in the **Label** text field.

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

4 Locate the **Plot Settings** section.

5 Select the **y-axis label** check box. In the associated text field, type `Conversion A (%)`.

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

Global 1

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

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

3 From the **Dataset** list, choose **Study 1/Adiabatic (sol2)**.

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>X_A - Conversion, A**.

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

6 Locate the **Legends** section. From the **Legends** list, choose **Manual**.

7 In the table, enter the following settings:

Legends
Adiabatic

Global 2

1 Right-click **Results>Conversion A (re)>Global 1** and choose **Duplicate**.

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

3 From the **Dataset** list, choose **Study 1/With heat exchange (sol3)**.

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

Legends
With heat exchange

5 In the **Conversion A (re)** toolbar, click **Plot**.

Last set up Figure 7 to plot the conversion of acetone with varied inlet molar fractions of inert for the adiabatic case.

Conversion A with inert (re)

1 In the **Model Builder** window, under **Results** click **1D Plot Group 5**.

2 In the **Settings** window for **1D Plot Group**, type `Conversion A with inert (re)` in the **Label** text field.

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

4 Locate the **Plot Settings** section.

5 Select the **x-axis label** check box. In the associated text field, type `Reactor volume (m<sup>3</sup>)`.

6 Select the **y-axis label** check box. In the associated text field, type `Conversion A (%)`.

7 Locate the **Legend** section. From the **Position** list, choose **Lower right**.

Global 1

1 Right-click **Conversion A with inert (re)** and choose **Global**.

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

3 From the **Dataset** list, choose **Study 1/With inert (sol8)**.

4 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Definitions>Variables>X_A - Conversion, A**.

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

6 Locate the **Legends** section. From the **Legends** list, choose **Evaluated**.

7 In the **Legend** text field, type `eval(A_frac*100) mol% A at inlet`.

8 In the **Conversion A with inert (re)** toolbar, click **Plot**.

Temperature (re) 1

In the **Model Builder** window, under **Results** right-click **Temperature (re) 1** and choose **Delete**.