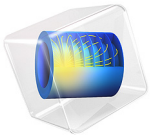

HI Batch Reactor

Introduction

The batch reactor is a widely used system for production of chemicals in various chemical industries. This reactor type together with the continuous stirred tank reactor (CSTR) and plug-flow reactor can be treated as ideal. In the case of the batch reactor, ideal conditions equal perfectly mixed conditions, meaning that temperature and compositions are the same throughout the reactor, and thus that the problem can be modeled in 0D.

In this example the isothermal and nonisothermal behaviors of the gaseous hydrogen iodine (HI) reaction are modeled in a perfectly mixed Batch reactor. The model utilizes the Batch reactor feature with constant volume within the Reaction Engineering interface of the Chemical Reaction Engineering Module.

Model Description

A classical example on reaction kinetics, namely the hydrogen iodine reaction (Ref. 1), is modeled. The reversible bimolecular reaction is here assumed to properly describe the kinetics:

$$\mathrm{H_2(g) + I_2(g) = 2HI(g)}$$

The model simulates experiments where an initially equimolar mixture of gas reacts. The reaction runs in a perfectly mixed batch reactor of constant volume. The balance equation for each species, i, that is solved in the Reaction Engineering interface is expressed as:

$$\frac{\mathrm{d}c_i}{\mathrm{d}t} = \sum_{j=1}^{n_r} \nu_{ij} r_j$$

where c_i is the concentration (SI unit: mol/m^3) and R_i the sum of the reaction rate contributions from each participating reaction (SI unit: mol/(m^{3}s)), which will give the production rate of species i. In this case we only have one reaction. Both isothermal and nonisothermal conditions are modeled. An energy balance for the Batch reactor is by default defined in the latter case, according to:

$$V_\mathrm{r} \sum_i c_i C_{p,i} \frac{\mathrm{d}T}{\mathrm{d}t} = Q + Q_\mathrm{ext} + V_\mathrm{r} \frac{\mathrm{d}p}{\mathrm{d}t}$$

where V_r denotes the reactor volume (SI unit: m^3), c_i is the species concentration (SI unit: mol/m^3), $C_{p,i}$ is the species molar heat capacity (SI unit: J/(mol·K)), T is the temperature (SI unit: K), and p the pressure (SI unit: Pa). On the right-hand side, Q is the heat due to

chemical reaction (SI unit: W), and Q_{ext} denotes heat added to the system (SI unit: W). The heat of reaction is calculated from the reactor volume, the molar enthalpy, H_i (J/mol), and the reaction rate, as given in the following equation:

$$Q = -V_r \sum_i H_i r_i$$

The results are used to compare the conditions and to determine the reaction's equilibrium constant at 700 K.

Results and Discussion

The concentration of the reactants and products for both reaction conditions are displayed in Figure 1. The reactant concentrations overlap. The plot shows that the reactor is close to steady state after roughly 36,000 s (10 hours) for the isothermal case. In the nonisothermal case, steady state is reached much faster, after approximately 2000 s.

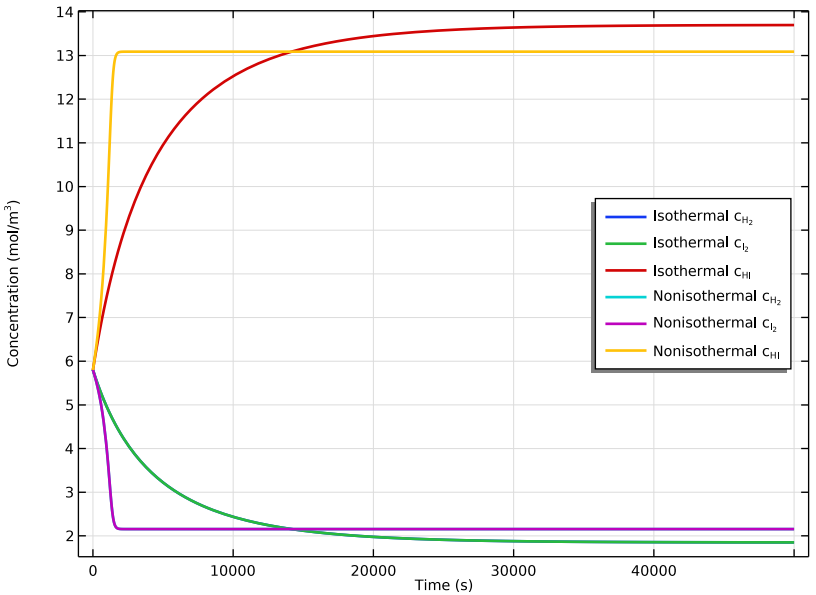

Figure 1: Reactant and product concentrations as functions of time for the isothermal and nonisothermal conditions.

The equilibrium quotient, K_Q, is monitored with the following relationship:

$$K_{\mathrm{Q}} = \frac{c_{\mathrm{HI}}^{2}}{c_{\mathrm{H_2}} c_{\mathrm{I_2}}}$$

which at steady state should yield the equilibrium constant. Figure 2 shows that the equilibrium expression asymptotically reaches the value of roughly 54.9 at isothermal conditions, which is also the relationship between k_{f} and k_{r} in the model.

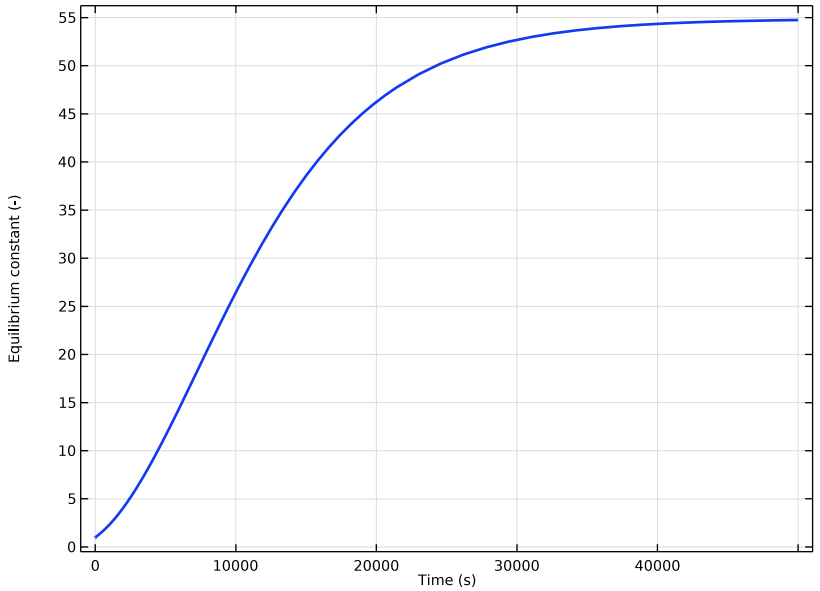

Figure 2: Equilibrium expression at isothermal conditions.

In Figure 3, the temperature is shown to increase 109 K to 809 K as steady state is reached.

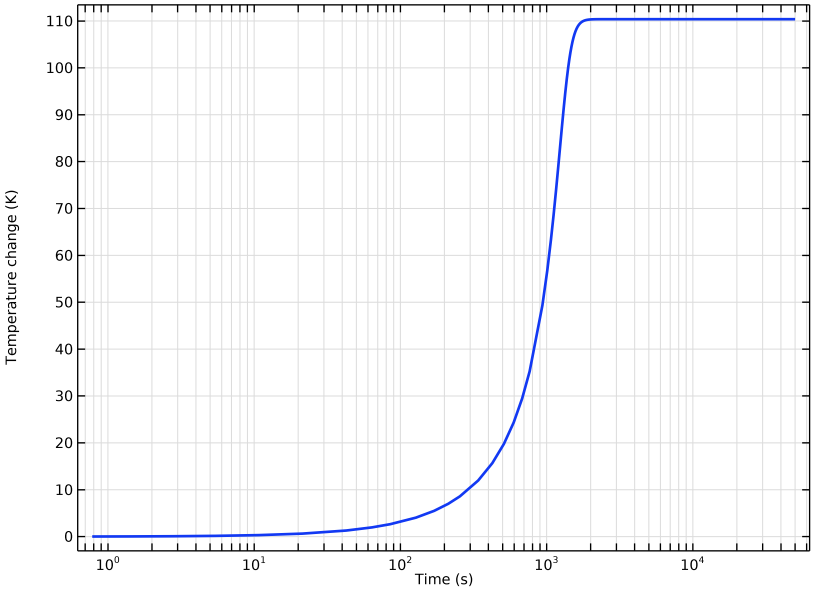

Figure 3: Reactor temperature as a function of time.

Figure 4 shows the heat of reaction for isothermal and adiabatic reactor.

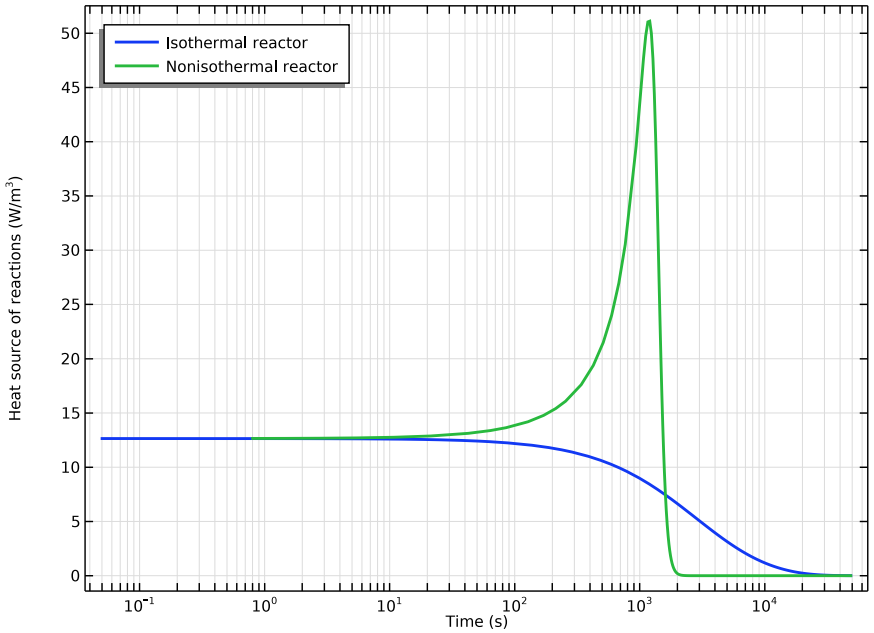

Figure 4: Heat of reaction for isothermal and adiabatic reactor.

Reference

1. J.H. Sullivan, "Mechanism of the 'Bimolecular' Hydrogen — Iodine Reaction," *J. Chem. Phys.*, vol. 46, p. 73, 1967.

Application Library path: `Chemical_Reaction_Engineering_Module/Thermodynamics/hi_batch_reactor`

Modeling Instructions

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**.

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 `hi_batch_reactor_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 Find the **Mass balance** subsection. In the V_r text field, type `V_reactor`.

4 Locate the **Energy Balance** section. In the T text field, type `Tinit`.

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 `H2+I2<=>2HI`.

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`.

7 In the A^r text field, type `Ar_reaction`.

8 In the E^r text field, type `Er_reaction`.

Initial Values 1

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

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

3 In the table, enter the following settings:

Species	Concentration (mol/m^3)
H2	cinit_H2
HI	cinit_HI
I2	cinit_I2

DEFINITIONS

Variables 1

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

Add some variables that need to be investigated. Note that since this is assumed to be an ideal solution, the expression for the equilibrium constant contains the concentration variables instead of the activities.

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 `hi_batch_reactor_variables.txt`.

5 In the **Reaction Engineering** toolbar, click **Thermodynamics** and choose **Thermodynamic System**.

SELECT SYSTEM

1 Go to the **Select System** window.

2 Click **Next** in the window toolbar.

SELECT SPECIES

1 Go to the **Select Species** window.

2 In the **Species** list, select **hydrogen iodide (10034-85-2, HI)**.

3 Click **Add Selected**.

4 In the **Species** list, select **hydrogen (1333-74-0, H2)**.

5 Click **Add Selected**.

6 In the **Species** list, select **iodine (7553-56-2, I2)**.

7 Click + **Add Selected**.

8 Click **Next** in the window toolbar.

SELECT THERMODYNAMIC MODEL

1 Go to the **Select Thermodynamic Model** window.

2 Click **Finish** in the window toolbar.

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**, click to expand the **Mixture Properties** section.

3 Select the **Thermodynamics** check box.

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

Species	From Thermodynamics
H2	H2
HI	HI
I2	I2

5 Locate the **Energy Balance** section. From the list, choose **Exclude**.

STUDY 1

Solve first for isothermal conditions.

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 In the **Output times** text field, type `0.5e5`.

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

STUDY 1

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**.

Isothermal

1 In the **Model Builder** window, right-click **Solution 1 - Copy 1 (sol2)** and choose **Rename**.

2 In the **Rename Solution** dialog box, type `Isothermal` in the **New label** text field.

3 Click **OK**.

Select nonisothermal settings in the **Reaction Engineering** interface.

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 From the list, choose **Include**.

Initial Values 1

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

Solve for nonisothermal conditions.

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**.

Nonisothermal

1 In the **Model Builder** window, right-click **Solution 1 - Copy 1 (sol3)** and choose **Rename**.

2 In the **Rename Solution** dialog box, type `Nonisothermal` in the **New label** text field.

3 Click **OK**.

RESULTS

Concentration (re)

1 In the **Model Builder** window, expand the **Results>Concentration (re)** node, then click **Concentration (re)**.

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

3 From the **Position** list, choose **Middle right**.

Global 1

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

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

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

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

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

6 In the table, enter the following settings:

Legends
Isothermal c_{H₂}
Isothermal c_{I₂}
Isothermal c_{HI}

7 Click to expand the **Coloring and Style** section. In the **Width** text field, type 2.

Global 2

1 Right-click **Results>Concentration (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/Nonisothermal (sol3)**.

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

Legends
Nonisothermal c_{H₂}
Nonisothermal c_{I₂}
Nonisothermal c_{HI}

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

Equilibrium constant

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

2 Right-click **1D Plot Group 2** and choose **Rename**.

3 In the **Rename 1D Plot Group** dialog box, type `Equilibrium constant` in the **New label** text field.

4 Click **OK**.

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

6 From the **Dataset** list, choose **Study 1/Isothermal (sol2)**.

7 Locate the **Plot Settings** section. Select the **x-axis label** check box.

8 In the associated text field, type `Time (s)`.

9 Select the **y-axis label** check box.

10 In the associated text field, type `Equilibrium constant (-)`.

Global 1

1 Right-click **Equilibrium constant** and choose **Global**.

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>K_equi - Equilibrium constant**.

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

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

5 Locate the **Coloring and Style** section. In the **Width** text field, type `2`.

6 In the **Equilibrium constant** toolbar, click **Plot**.

Temperature change

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

2 Right-click **1D Plot Group 3** and choose **Rename**.

3 In the **Rename 1D Plot Group** dialog box, type `Temperature change` in the **New label** text field.

4 Click **OK**.

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

6 From the **Dataset** list, choose **Study 1/Nonisothermal (sol3)**.

7 Locate the **Plot Settings** section. Select the **x-axis label** check box.

8 In the associated text field, type `Time (s)`.

9 Select the **y-axis label** check box.

10 In the associated text field, type `Temperature change (K)`.

11 Click the **x-Axis Log Scale** button in the **Graphics** toolbar.

Global 1

1 Right-click **Temperature change** and choose **Global**.

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>T_change - Temperature change - K**.

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

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

5 Locate the **Coloring and Style** section. In the **Width** text field, type 2.

6 In the **Temperature change** toolbar, click **Plot**.

Heat of reaction

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

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

3 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Global 1

1 Right-click **Heat of reaction** and choose **Global**.

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

3 Click **Clear Table**.

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.Qheat - Heat source of reactions - W/m³**.

5 Click to expand the **Coloring and Style** section. In the **Width** text field, type 2.

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

7 In the table, enter the following settings:

Legends
`Isothermal reactor`

8 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Isothermal (sol2)**.

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

Global 2

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

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

3 In the table, enter the following settings:

Legends
`Nonisothermal reactor`

4 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Nonisothermal (sol3)**.

Heat of reaction

1 In the **Model Builder** window, click **Heat of reaction**.

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

3 Select the **x-axis log scale** check box.

4 In the **Heat of reaction** toolbar, click  **Plot**.