Created in COMSOL Multiphysics 6.2

Ideal Stirred Tank Reactor System

Introduction

In the chemical and biochemical industries, for instance in fermentation processes, reactors having well-mixed conditions and liquid level control are common.

This example shows how to use the Reaction Engineering interface to model a 0D ideal system of tank reactors in series, with controlled feed inlet and product outlet streams. The volume change in each reactor is monitored and controlled.

Model Definition

This model solves for a liquid-phase first order irreversible reaction $A \rightarrow B$ where

$$r = kc_A \tag{1}$$

In Equation 1, r is the reaction rate (SI unit: mol/(m^3·s)), k is the rate constant (SI unit: 1/s), and c_A is the concentration of A.

The reaction takes place in a system of two ideal reactors in series. The first reactor tank has a volume capacity of $v_{\mathrm{tank1}} = 1\ \mathrm{m}^3$ and the second $v_{\mathrm{tank2}} = 1.5\ \mathrm{m}^3$ initially.

Initially the reactors are charged only with solvent. A is fed with solvent to the first tank with a volumetric flow rate of $v_{\mathrm{f1}} = 1\ \mathrm{m}^3/\mathrm{min}$. The volumetric flow rate at the outlet of the first tank is set to $v_{\mathrm{out1}} = 0.9\ \mathrm{m}^3/\mathrm{min}$. This whole stream is fed to the second tank in the system, $v_{\mathrm{f2}} = v_{\mathrm{out1}}$. The second tank also has a fresh supply of A with solvent entering at a rate of $v_{\mathrm{f2}} = 0.5\ \mathrm{m}^3/\mathrm{min}$. In a similar way as for the first reactor, the outlet flow is also set to $v_{\mathrm{out2}} = 1\ \mathrm{m}^3/\mathrm{min}$. Figure 1 shows the reactor system in detail.

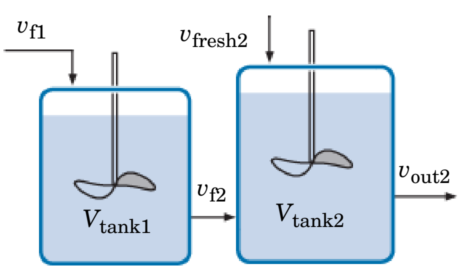

Figure 1: The reactor system.

The mass balance for species i in each reactor is shown in Equation 2:

$$\frac{d(V_r c_i)}{dt} = \sum_j v_{\mathrm{f},j}\, c_{\mathrm{f},ij} - \sum_k v_{\mathrm{out},k}\, c_i + R_i V_r \quad (2)$$

V_r denotes the reactor volume (SI unit: m^3), R_i is the species rate expression (SI unit: $mol/(m^3 \cdot s)$). Subscripts f and **out** indicate the feed inlet and the outlet, respectively. j and k are the number of feed inlet and outlet streams, respectively.

The volume depends on the volumetric production rate v_p and the regulated inlet and outlet volumetric flow rates as shown in Equation 3:

$$\frac{dV_r}{dt} = \sum_j v_{\mathrm{f},j} - \sum_k v_{\mathrm{out},k} + v_p \quad (3)$$

The model incorporates two stop conditions: If any of the reactor volumes is 1 % or less of the initial volumes, the computations stop.

Results and Discussion

In Figure 2 and Figure 3, the concentrations of the species in the two tanks are shown.

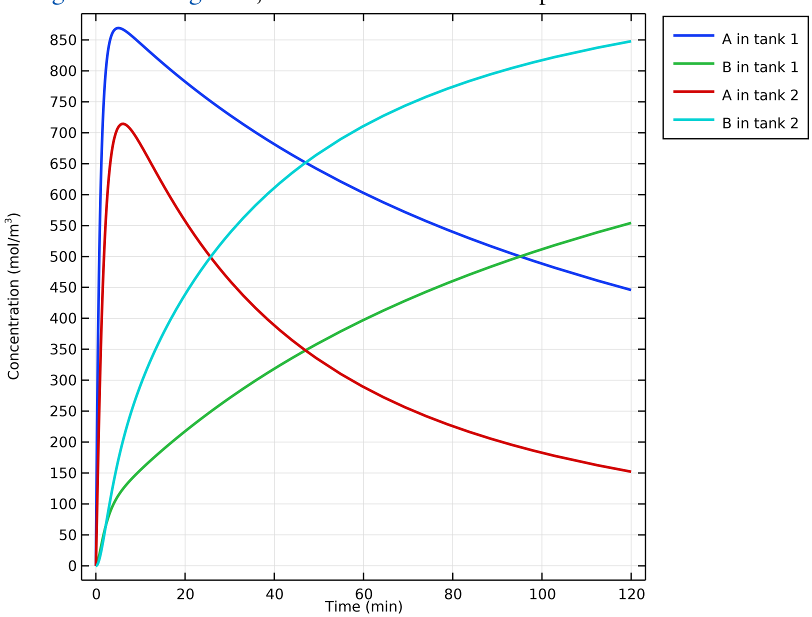

Figure 2: Concentrations of A and B in tank 1 and tank 2.

The variation of the tank volumes is shown in Figure 3. With a known diameter of the reactor, the liquid level can be calculated from this volume. Given the inlet and outlet flows, this system will fill up the tanks considerably.

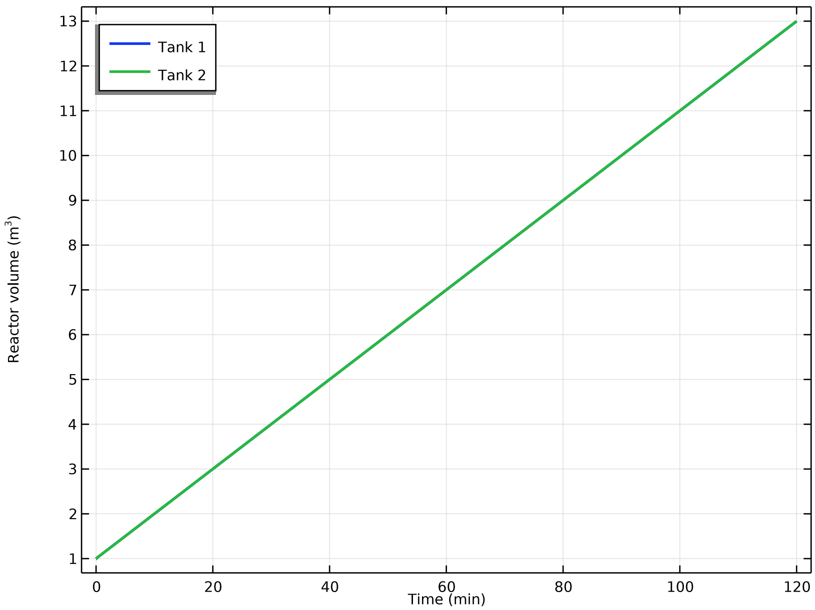

Figure 3: Tank volumes.

The results show only some system aspects that can be investigated with the Reaction Engineering interface. This application can also be utilized as a starting point for studying, for instance, startup and steady-state process conditions.

Application Library path: `Chemical_Reaction_Engineering_Module/Ideal_Tank_Reactors/tank_flow_system`

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 global parameters by importing their definitions from a data text file.

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 `tank_flow_system_parameters.txt`.

Start with the first reactor. Select the **CSTR constant mass/generic** reactor type to model the first reactor.

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 **CSTR, constant mass/generic**.
4 Locate the **Mixture Properties** section. From the **Phase** list, choose **Liquid**.

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=>B`.
4 Click **Apply**.
5 Locate the **Rate Constants** section. In the k^{f} text field, type `kf_reaction`.

Species: A

1. In the **Model Builder** window, click **Species: A**.
2. In the **Settings** window for **Species**, locate the **Chemical Formula** section.
3. In the M text field, type `Mn_A`.

Species: B

1. In the **Model Builder** window, click **Species: B**.
2. In the **Settings** window for **Species**, locate the **Chemical Formula** section.
3. In the M text field, type `Mn_B`.

Add a solvent (water) to the first tank.

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 `S`.
4. Locate the **Type** section. From the list, choose **Solvent**.
5. Locate the **Chemical Formula** section. In the M text field, type `Mn_S`.
6. In the ρ text field, type `density_S`.

   Generic in the **Mass Balance** section substitutes the constant mass condition. Choose this to set a constant value of the volumetric outlet rate, `v`.
7. In the **Model Builder** window, click **Reaction Engineering (re)**.
8. In the **Settings** window for **Reaction Engineering**, locate the **Reactor** section.
9. Find the **Mass balance** subsection. From the **Volumetric rate** list, choose **Generic**.
10. Click **Reset to Default**.
11. In the v text field, type `v_outlet1`.

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 V_{r0} text field, type `Vr_init_tank1`.

   Set only solvent in the first tank initially.

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

Species	Concentration (mol/m^3)
S	`cinit_S`

Feed Inlet 1

Add one **Feed Inlet** stream to the first tank.

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

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

3 In the v_f text field, type `v_inlet`.

4 Locate the **Feed Inlet Concentration** section. In the **Feed inlet concentration** table, enter the following settings:

Species	Concentration (mol/m^3)
A	`cinlet_A1`
S	`cinlet_S`

5 In the **Model Builder** window, right-click **Reaction Engineering (re)** and choose **Copy**.

COMPONENT 1 (COMP1)

In the **Model Builder** window, right-click **Component 1 (comp1)** and choose **Paste Reaction Engineering**.

REACTION ENGINEERING 2 (RE2)

1 In the **Messages from Paste** dialog box, click **OK**.

Duplicating the first reactor and changing the necessary parameters that distinguishes the first from the second reactor.

2 In the **Model Builder** window, under **Component 1 (comp1)** click **Reaction Engineering 2 (re2)**.

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

4 Find the **Mass balance** subsection. In the v text field, type `v_outlet2`.

Initial Values 1

1 In the **Model Builder** window, expand the **Reaction Engineering 2 (re2)** node, then click **Initial Values 1**.

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

3 In the V_{r0} text field, type `Vr_init_tank2`.

The **Feed Inlet** stream to the second reactor is equal to the whole outlet stream from the first reactor.

Feed Inlet 1 - from Tank 1

1 In the **Model Builder** window, click **Feed Inlet 1**.

2 In the **Settings** window for **Feed Inlet**, type `Feed Inlet 1 - from Tank 1` in the **Label** text field.

3 Locate the **Feed Inlet Properties** section. In the v_f text field, type `v_outlet1`.

4 Locate the **Feed Inlet Concentration** section. In the **Feed inlet concentration** table, enter the following settings:

Species	Concentration (mol/m^3)
A	`re.c_A`
B	`re.c_B`
S	`re.c_S`

Feed Inlet 2 - Fresh

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

Add a second **Feed Inlet** stream to the second reactor to model the fresh feed.

2 In the **Settings** window for **Feed Inlet**, type `Feed Inlet 2 - Fresh` in the **Label** text field.

3 Locate the **Feed Inlet Properties** section. In the v_f text field, type `v_fresh2`.

4 Locate the **Feed Inlet Concentration** section. In the **Feed inlet concentration** table, enter the following settings:

Species	Concentration (mol/m^3)
A	`cfresh2_A`
S	`cinlet_S`

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 **min**.

4 In the **Output times** text field, type `range(0,0.1,120)`.

Solution 1 (sol1)

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

Stop the computations if any of the two reactor volumes is empty.

2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.

3 Right-click **Study 1>Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1** and choose **Stop Condition**.

4 In the **Settings** window for **Stop Condition**, locate the **Stop Expressions** section.

5 Click **Add**.

6 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.re.Vr<=Vr_init_tank1*0.01`	True (>=1)	√	`Stop expression 1`

7 Click **Add**.

8 In the table, enter the following settings:

Stop expression	Stop if	Active	Description
`comp1.re2.Vr<=Vr_init_tank2*0.01`	True (>=1)	√	`Stop expression 2`

9 Locate the **Output at Stop** section. From the **Add solution** list, choose **Steps before and after stop**.

10 Clear the **Add warning** check box.

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

RESULTS

Concentrations in Tanks

Follow these steps to create Figure 2.

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

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

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

Tank 1

1 In the **Model Builder** window, expand the **Concentrations in Tanks** node, then click **Global 1**.

2 In the **Settings** window for **Global**, type `Tank 1` in the **Label** text field.

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

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

5 In the table, enter the following settings:

Legends
`A in tank 1`
`B in tank 1`

6 Right-click **Tank 1** and choose **Duplicate**.

Tank 2

1 In the **Model Builder** window, under **Results>Concentrations in Tanks** click **Tank 1.1**.

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

3 Click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering 2>re2.c_A - 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 2>re2.c_B - Concentration - mol/m³**.

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

Legends
`A in tank 2`
`B in tank 2`

6 In the **Concentrations in Tanks** toolbar, click **Plot**.

Follow these steps to create Figure 3.

Volume in Tanks

1 In the **Model Builder** window, under **Results** click **Concentration (re2)**.

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

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

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

Tank 1

1 In the **Model Builder** window, expand the **Volume in Tanks** node, then click **Global 1**.

2 In the **Settings** window for **Global**, type `Tank 1` in the **Label** text field.

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.Vr - Reactor volume - m³**.

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

5 Locate the **Legends** section. Find the **Include** subsection. Select the **Label** check box.

6 Clear the **Solution** check box.

7 Clear the **Expression** check box.

8 Right-click **Tank 1** and choose **Duplicate**.

Tank 2

1 In the **Model Builder** window, under **Results>Volume in Tanks** click **Tank 1.1**.

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

3 In the **Volume in Tanks** toolbar, click **Plot**.