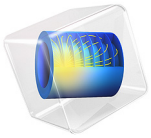

Model created in COMSOL Multiphysics 6.4

Tank Series with Feedback Control

Introduction

This example illustrates a series of three consecutive CSTR reactors. A feedback loop continuously adjusts the inlet concentration of the first tank to keep the concentration at the outlet of the last reactor close to a set level. The model utilizes the Reaction Engineering interface in the Chemical Reaction Engineering Module.

Model Description

The following example reproduces the results in Ref. 1. Three CSTR reactors are connected in a series arrangement, as in Figure 1.

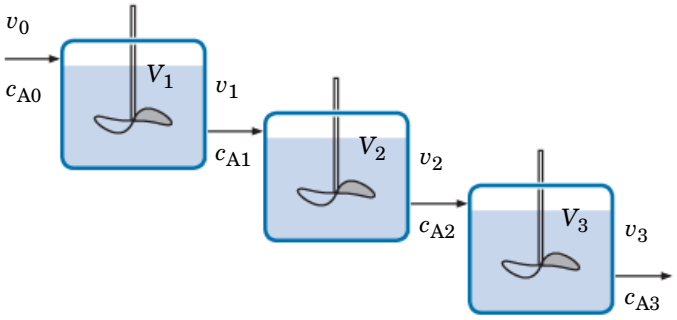

Figure 1: An example of three continuous stirred tank reactors (CSTRs) in a series.

The same unimolecular liquid reaction takes place in aqueous solution in each unit:

$$\mathrm{A} \xrightarrow{k} \mathrm{B}$$

Under isothermal conditions and the assumption that the volume is constant, the balance equations for reactant A in each of the tanks become:

$$V_1 \frac{dc_{A1}}{dt} = v_0 c_{A0} - v_1 c_{A1} - V_1 k c_{A1}$$

$$V_2 \frac{dc_{A2}}{dt} = v_1 c_{A1} - v_2 c_{A2} - V_2 k c_{A2}$$

$$V_3 \frac{dc_{A3}}{dt} = v_2 c_{A2} - v_3 c_{A3} - V_3 k c_{A3}$$

V denotes the reactor volume (SI unit: m^3) and v is the volumetric flow rate for an inlet or outlet (SI unit: m^3/s). The concentration of A is represented by c_A (SI unit: mol/m^3), while k is the rate constant (SI unit: $1/s$).

These equations are modeled using the CSTR reactor with constant volume feature in the Reaction Engineering interface. The feed inlet streams connect the reactors to each other. It is assumed that the reactor holdups (volumes) are constant and that the reacting fluid has constant density. Thus, all volumetric flow rates are equal within the reactor system:

$$v_0 = v_1 = v_2 = v_3 = v$$

In this case the volumetric flow rate of the system is 8 l/s. This implies that the residence time of each reactor, assuming perfect mixing, is

$$\tau = \frac{V}{v} = \frac{1}{8 \cdot 10^{-3}} = 125 \text{ s}$$

FEEDBACK CONTROL

The model also considers adding a feedback control to the system where the concentration of A in the outlet stream leaving the third tank, c_{A3}, is monitored. Adjustments are made to the inlet concentration of the first tank c_{A0} to keep c_{A3} close to a set level, c_{A3}^{set}. Figure 2 illustrates the control system.

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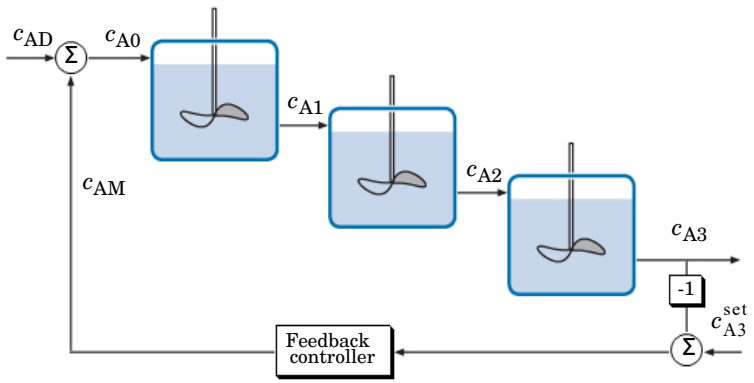

Figure 2: An example of tanks in a series with feedback control.

The concentration of A in the inlet to the first reactor is now given by:

$$c_{A0} = c_{AM} + c_{AD}$$

The variable c_{AD} is a disturbance concentration while c_{AM} is the manipulated concentration changed by the controller. The value of c_{AM} is based on the magnitude of the error and the integral of the error according to this expression:

$$c_{AM} = 800\frac{\text{mol}}{\text{m}^3} + K_c\left(E + \frac{1}{\tau_i}\int E dt\right) \quad (1)$$

Above, the error is defined by:

$$E = c_{A3}^{\text{set}} - c_{A3}$$

where K_c is the controller gain and τ_i the controller reset time. The term 800 mol/m^3 in Equation 1 is the bias value of the controller, that is, the value of c_{AM} at time zero.

According to Equation 1, the integral of the error needs to be evaluated for the feedback control. Noting that from:

$$\frac{d}{dt}\left(\int E dt\right) = E$$

it is clear that the integral can be evaluated by solving an ODE. The ODE is specified by adding a Global Equation, a Global ODEs and PDEs interface, to the model.

Results

Figure 3 shows the concentration of A (SI unit: mol/m^3) in the three tanks as a function of time (SI unit: s). The initial concentration of A is 400 mol/m^3 in tank 1, 200 mol/m^3

in tank 2, and 100 mol/m^3 in tank 3. The system is "open loop," that is, without feedback control. The reactors reach steady state after approximately 10 minutes.

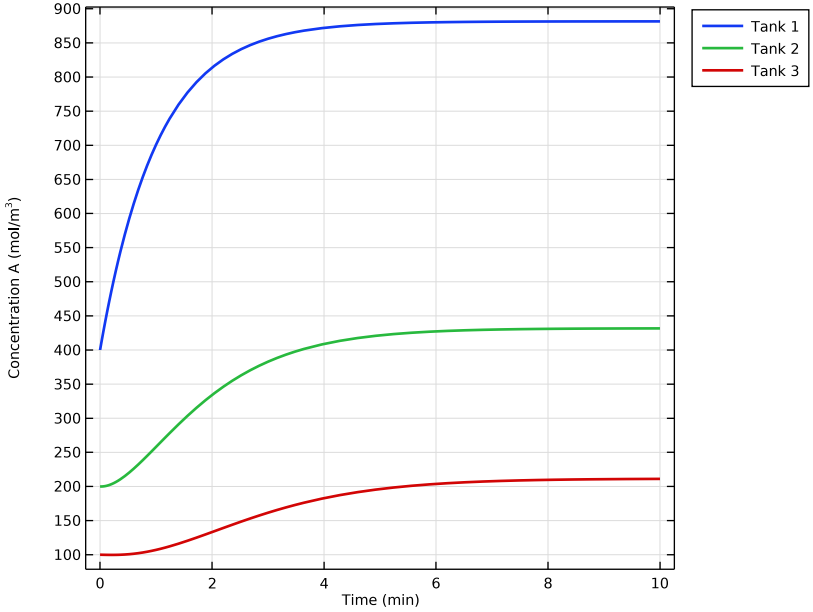

Figure 3: Concentration transients for three tanks in series without feedback control.

Figure 4 illustrates the concentration transients in the "closed loop" system. The control system, regulating on the outlet concentration in the last unit, sets the inlet concentration of the first unit.

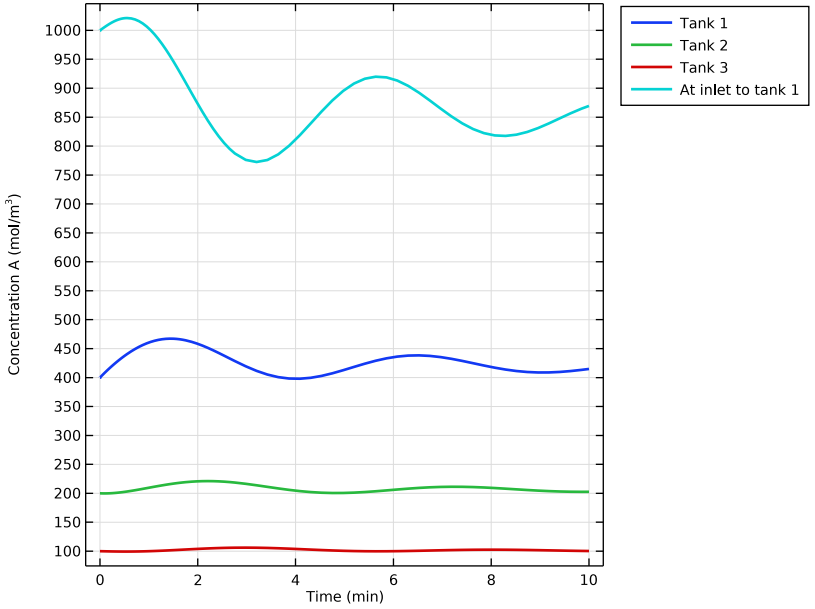

Figure 4: Concentration transients for three tanks in series with feedback control. c_{AM} is the manipulated concentration.

The set concentration, c_{A3}^{set}, is 100 mol/m^3. The feedback control appears to be reasonably tuned to keep the outlet concentration from tank 3 at the desired level.

Reference

1. W.L. Luyben, *Process Modeling, Simulation and Control for Chemical Engineers* 2nd ed., McGraw Hill, pp. 119–124, 1990.

Application Library path: `Chemical_Reaction_Engineering_Module/Ideal_Tank_Reactors/tankinseries_control`

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.

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 `tankinseries_control_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**, type `tank1` in the **Name** text field.

The interface name will help you keep track of the variables that belong to the physics interface. In this case, the **Reaction Engineering** interface corresponds to a tank reactor, and to keep this in mind the interface name is changed to `Tank 1`.

3 Locate the **Reactor** section. From the **Reactor type** list, choose **CSTR, constant volume**.

4 Find the **Mass balance** subsection. In the V_r text field, type `Vr_tank`.

5 Click to expand 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 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`.

4 In the ρ text field, type `rho_spec`.

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`.

4 In the ρ text field, type `rho_spec`.

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 `H2O`.

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

5 Locate the **Chemical Formula** section. In the M text field, type `Mn_solv`.

6 In the ρ text field, type `rho_solv`.

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)
A	`cinit_A_tank1`
H2O	`c_solv`

Feed Inlet 1

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

The volumetric flow is constant in the tank.

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

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

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

Species	Concentration (mol/m^3)
A	`cinlet_A`
H2O	`c_solv`

5 In the **Model Builder** window, right-click **Reaction Engineering (tank1)** and choose **Copy**.

REACTION ENGINEERING 2 (TANK2)

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

2 In the **Messages from Paste** dialog, click **OK**.

Initial Values 1

1 In the **Model Builder** window, expand the **Reaction Engineering 2 (tank2)** node, then 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)
A	`cinit_A_tank2`

Feed Inlet 1

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

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

3 In the table, enter the following settings:

Species	Concentration (mol/m^3)
A	`tank1.c_A`
B	`tank1.c_B`

4 In the **Model Builder** window, right-click **Reaction Engineering 2 (tank2)** and choose **Copy**.

REACTION ENGINEERING 3 (TANK3)

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

2 In the **Messages from Paste** dialog, click **OK**.

Initial Values 1

1 In the **Model Builder** window, expand the **Reaction Engineering 3 (tank3)** node, then 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)
A	`cinit_A_tank3`

Feed Inlet 1

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

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

3 In the table, enter the following settings:

Species	Concentration (mol/m^3)
A	`tank2.c_A`
B	`tank2.c_B`
H2O	`c_solv`

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 In the **Output times** text field, type `range(0,1,600)`.

4 In the **Model Builder** window, click **Study 1**.

5 In the **Settings** window for **Study**, locate the **Study Settings** section.

6 Clear the **Generate default plots** checkbox.

7 Clear the **Generate convergence plots** checkbox.

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

Store a copy of the solution for the open loop reactor system. This way you readily access the results for comparison with the closed loop system.

Solver Configurations

Click **Create Solution Copy**.

Open Loop

1 In the **Model Builder** window, expand the **Solver Configurations** node, then click **Solution 1 - Copy 1 (sol2)**.

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

Follow the steps below to plot the concentration of species A in all three tanks for the open loop system.

RESULTS

Open Loop

1 In the **Results** toolbar, click **1D Plot Group**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Open Loop (sol2)**.

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

5 Locate the **Plot Settings** section.

6 Select the **y-axis label** checkbox. In the associated text field, type `Concentration A (mol/m<sup>3</sup>)`.

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

Global 1

1 Right-click **Open Loop** 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)** > **Reaction Engineering** > **tank1.c_A - 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 2** > **tank2.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 3** > **tank3.c_A - Concentration - mol/m³**.

5 Locate the **x-Axis Data** section. From the **Parameter** list, choose **Expression**.

6 In the **Expression** text field, type `t`.

7 From the **Unit** list, choose **min**.

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

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

10 In the table, enter the following settings:

Legends
Tank 1
Tank 2
Tank 3

11 In the **Open Loop** toolbar, click **Plot**.

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

COMPONENT 1 (COMP1)

Set up the feedback control to model the closed loop system using the **Global ODEs and PDEs** interface and some variables.

ADD PHYSICS

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

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

3 In the tree, select **Mathematics** > **ODE and DAE Interfaces** > **Global ODEs and DAEs (ge)**.

4 Click the **Add to Component 1** button in the window toolbar.

5 In the **Home** toolbar, click **Add Physics** to close the **Add Physics** window.

GLOBAL ODES AND DAES (GE)

Global Equations 1 (ODE7)

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Global ODEs and DAEs (ge)** click **Global Equations 1 (ODE7)**.

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

3 In the table, enter the following settings:

Name	f(u,ut,utt,t) (1)	Initial value (u_0) (1)	Initial value (ut_0) (1/s)	Description
E_int	E_intt-E	0	0	

4 Locate the **Units** section. Click **Define Dependent Variable Unit**.

5 In the **Dependent variable quantity** table, enter the following settings:

Dependent variable quantity	Unit
Custom unit	`mol/m^3*s`

6 Click **Select Source Term Quantity**.

7 In the **Physical Quantity** dialog, type `concentration` in the text field.

8 In the tree, select **General** > **Concentration (mol/m^3)**.

9 Click **OK**.

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
`E`	`cset_A-tank3.c_A`	mol/m³	`Measured error`
`cM_A`	`800+Kc*(E+E_int/tau1)`	mol/m³	`Manipulated concentration`
`cinlet_A`	`max((cM_A+cdisturb_A), 0)`	mol/m³	`Inlet concentration`

STUDY 1

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

Close Loop

1 In the **Model Builder** window, under **Study 1** > **Solver Configurations** click **Solution 1 (sol1)**.

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

Follow the steps below to plot the concentration of species A in all three tanks and at the inlet for the closed loop system.

RESULTS

Closed Loop

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

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Close Loop (sol1)**.

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

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

Global 1

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

2 In the **Settings** window for **Global**, click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component 1 (comp1)** > **Definitions** > **Variables** > **cinlet_A - Inlet concentration - mol/m³**.

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

Legends
Tank 1
Tank 2
Tank 3
At inlet to tank 1

4 In the **Closed Loop** toolbar, click **Plot**.

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