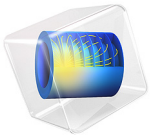

Parameter Estimation for Nonideal Reactor Models

Introduction

Real reactors can be modeled as combinations of ideal reactors. In this example, the "Dead zone model" is utilized. Two ideal CSTRs with interchange are used to model a real reactor. One CSTR represents the highly agitated region and the other one the less agitated region. Two parameters relating the volume and exchange rate of the two regions are required for this. The parameters are found by comparing the model results to experimental tracer data. Applying the Parameter Estimation feature in the Reaction Engineering interface makes this an easy task.

A problem description similar to the model presented here is given in Ref. 1.

Note: This application requires the Optimization Module and the Chemical Reaction Engineering Module.

Model Definition

Two ideal CSTRs with interchange capture the essential behavior of a real reactor system.

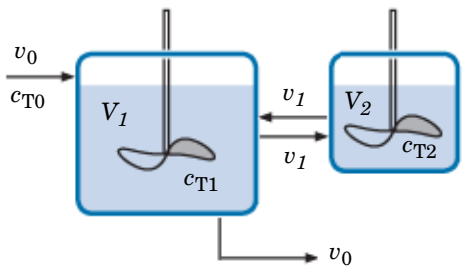

Figure 1: A real reactor can be modeled by two ideal CSTRs with interchange.

The highly agitated volume is represented by V_1 and the less agitated region by V_2. The total real reactor volume is defined as:

$$V = V_1 + V_2 \tag{1}$$

and the parameter α gives the fraction of the total volume that belongs to V_1:

$$V_1 = \alpha V$$

Fluid is exchanged between volumes at a rate of v_1 (SI unit: m^3/s), and the parameter β relates this rate to the inlet flow rate:

$$v_1 = \beta v_0$$

Assuming that the reactor volume is constant, then the space time, τ (SI unit: s), is:

$$\tau = \frac{V}{v_0}$$

MASS BALANCES

To evaluate the parameters α and β, a tracer compound is added through the reactor inlet stream, after which a response curve is measured at the outlet. Mass balances over the two CSTRs provide a model to which the experimental data can be compared. The mass balances are:

$$V_1 \frac{dc_{T1}}{dt} = v_0 c_{T0} + v_1 c_{T2} - v_0 c_{T1} - v_1 c_{T1}$$

$$V_2 \frac{dc_{T2}}{dt} = v_1 c_{T1} - v_1 c_{T2}$$

where c_{T1} is the tracer concentration (SI unit: mol $/m^3$) in the region given by V_1, and c_{T2} is the tracer concentration in V_2. c_{T0} is the tracer amount into the real reactor. The tracer compound is said to be diluted in water.

This coupled set of ODEs can easily be set up by combining two Reaction Engineering interfaces where the reactor type is set to **CSTR constant mass/generic**.

EXPERIMENTAL DATA

An experiment is performed where a 1000 mol/m^3 tracer solution is added in the reactor feed inlet stream. The tracer concentration in the reactor outlet stream is then recorded as a function of time. The data is presented in Table 1 below.

TABLE 1: EXPERIMENTAL DATA.

TIME (S)	CONCENTRATION (MOL/M3)
600	242
1200	446
1800	585
2400	668

TABLE 1: EXPERIMENTAL DATA.

TIME (S)	CONCENTRATION (MOL/M3)
3600	795
6000	909
9000	953
18000	991
24000	994

The Parameter Estimation feature accepts *comma-separated value* files (*csv*-files) for import of experimental data into the software. After import, the columns of the data file are shown and are mapped to the model variables.

Results and Discussion

Figure 2 shows the model results, both when using an initial guess, and when using parameter estimation. The figure also shows the experimental data. The results from the parameter estimation are seen to coincide well with the experimental data.

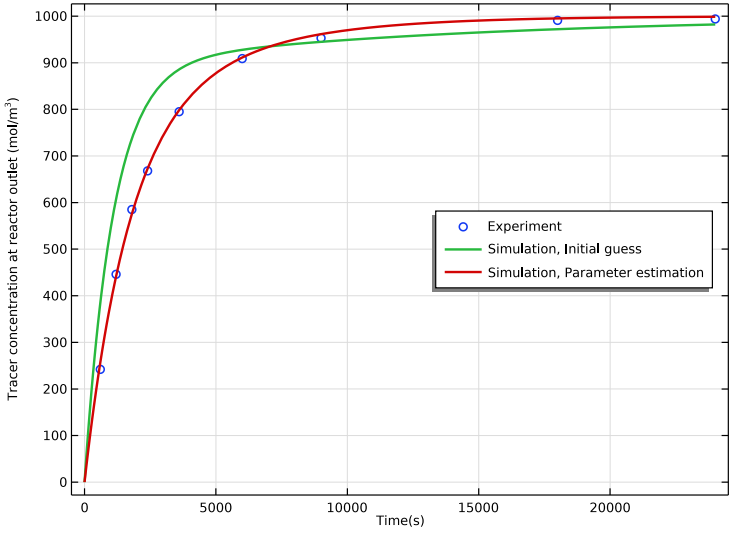

Figure 2: Model results and experimental data of the tracer concentration in the real reactor outlet.

The estimated values of α and β are 0.83 and 0.11, respectively.

Reference

1. H.S. Fogler, *Elements in Chemical Reaction Engineering*, 4th ed., Prentice Hall, pp. 985–987, 2005.

Application Library path: `Chemical_Reaction_Engineering_Module/Tutorials/nonideal_cstr`

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 **Applications 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 `nonideal_cstr_parameters.txt`.

Start defining the first CSTR representing the highly agitated zone.

REACTION ENGINEERING - CSTR 1

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

2 In the **Settings** window for **Reaction Engineering**, type `Reaction Engineering - CSTR 1` in the **Label** text field.

3 In the **Name** text field, type `re1`.

4 Locate the **Reactor** section. From the **Reactor type** list, choose **CSTR, constant mass/ generic**.

5 Locate the **Mixture Properties** section. From the **Phase** list, choose **Liquid**.

6 Locate the **Reactor** section. Find the **Mass balance** subsection. From the **Volumetric rate** list, choose **Generic**.

Two streams are assumed to exit the first CSTR: `v0` and `v0*`beta.

7 In the v text field, type `(1+beta)*v0`.

Species 1

1 In the **Reaction Engineering** toolbar, click **Species**.

2 In the **Settings** window for **Species**, locate the **Species Name** section.

3 In the text field, type `T`.

4 In the **Reaction Engineering** toolbar, click **Species**.

Species 1

1 In the **Settings** window for **Species**, locate the **Species Name** section.

2 In the text field, type `H2O`.

3 Locate the **Species Type** section. From the list, choose **Solvent**.

Species: T

1 In the **Model Builder** window, click **Species: T**.

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

3 In the M text field, type `Mn_T`.

Species: H2O

1 In the **Model Builder** window, click **Species: H2O**.

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

3 In the M text field, type `Mn_w`.

4 In the ρ text field, type `rho_w`.

Initial Values 1

The first CSTR has an initial volume alpha times the total real reactor volume.

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 `alpha*Vtot`.

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

Species	Concentration (mol/m^3)
H2O	c_w

Add two feed inlet streams to the first CSTR. One representing the flow entering the real reactor, v0, and another one representing the stream from the second CSTR, `v0*`beta.

Feed Inlet 1

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 `v0`.

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

Species	Concentration (mol/m^3)
H2O	c_w
T	c_T0

Feed Inlet 2

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 `v0*beta`.

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

Species	Concentration (mol/m^3)
H2O	c_w
T	re2.c_T

Continue to define the second CSTR representing the dead zone. To do this copy the first interface.

5 In the **Model Builder** window, right-click **Reaction Engineering - CSTR 1 (re1)** and choose **Copy**.

REACTION ENGINEERING - CSTR 2

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

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

3 In the **Settings** window for **Reaction Engineering**, type `Reaction Engineering - CSTR 2` in the **Label** text field.

Only one stream exits the second CSTR: `v0*`beta.

4 Locate the **Reactor** section. Find the **Mass balance** subsection. In the v text field, type `v0*beta`.

Initial Values 1

The second CSTR has an initial volume (1-alpha) times the total real reactor volume.

1 In the **Model Builder** window, expand the **Component 1 (comp1)>Reaction Engineering - CSTR 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 `(1-alpha)*Vtot`.

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

Species	Concentration (mol/m^3)
H2O	`c_w`

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 Properties** section.

3 In the v_f text field, type `v0*beta`.

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

Species	Concentration (mol/m^3)
T	`re1.c_T`

Remove the second feed inlet stream.

Feed Inlet 2

In the **Model Builder** window, right-click **Feed Inlet 2** and choose **Delete**.

REACTION ENGINEERING - CSTR 1 (RE1)

Now add a **Parameter Estimation** feature to be used in the optimization.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Reaction Engineering - CSTR 1 (re1)**.

Parameter Estimation 1

1 In the **Reaction Engineering** toolbar, click  **Parameter Estimation**.

2 In the **Settings** window for **Parameter Estimation**, locate the **Estimation Parameters** section.

3 In the **Parameter** table, enter the following settings:

Parameter	Initial value	Scale	Lower bound	Upper bound
alpha	0.5	1		

4 Click + **Add**.

5 In the **Parameter** table, enter the following settings:

Parameter	Initial value	Scale	Lower bound	Upper bound
beta	0.1	1		

Experiment 1

1 In the **Reaction Engineering** toolbar, click  **Attributes** and choose **Experiment**.

Read in the csv-file with the **Experimental Data** and map the data columns with the model variables.

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

3 Click **Browse**.

4 Browse to the model's Application Libraries folder and double-click the file `nonideal_cstr_data.csv`.

5 Click **Import**.

6 In the table, enter the following settings:

Data column	Use	Model variables	Unit	Weight
Tracer (mol/m3)	√	c_T	1	1

Solve the model using the initial values of the alpha and beta parameters.

STUDY 1: INITIAL GUESS

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

2 In the **Settings** window for **Study**, type `Study 1: Initial guess` in the **Label** text field.

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1: Initial guess** 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 `24000`.

Disable the **Parameter Estimation** feature for this study step.

4 Locate the **Physics and Variables Selection** section. Select the **Modify model configuration for study step** check box.

5 In the **Physics and variables selection** tree, select **Component 1 (comp1)>Reaction Engineering - CSTR 1 (re1)>Parameter Estimation 1**.

6 Click **Disable**.

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

The following instructions generate Figure 2.

RESULTS

Concentration in Real Reactor

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

2 In the **Settings** window for **1D Plot Group**, type `Concentration in Real Reactor` in the **Label** text field.

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

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

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

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

7 In the associated text field, type `Tracer concentration at reactor outlet (mol/m<sup>3</sup>)`.

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

Experiment

1 In the **Model Builder** window, expand the **Concentration in Real Reactor** node, then click **Experiment 1 Data**.

2 In the **Settings** window for **Table Graph**, type `Experiment` in the **Label** text field.

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

4 In the table, enter the following settings:

Legends
Experiment

Simulation, Initial guess

1 In the **Model Builder** window, right-click **Concentration in Real Reactor** and choose **Global**.

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

3 From the **Dataset** list, choose **Study 1: Initial guess/Solution 1 (sol1)**.

4 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description

5 In the **Label** text field, type `Simulation, Initial guess`.

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

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

8 In the table, enter the following settings:

Legends
Simulation, Initial guess

9 In the **Concentration in Real Reactor** toolbar, click **Plot**.

The following instructions generate a figure with tracer concentrations in the two CSTRs.

Concentrations in CSTRs

1 In the **Model Builder** window, under **Results** click **Concentration (re1)**.

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

3 Locate the **Plot Settings** section. Select the **y-axis label** check box.

4 In the associated text field, type `Tracer concentrations (mol/m<sup>3</sup>)`.

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

Global 1

1 In the **Model Builder** window, expand the **Concentrations in CSTRs** 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)> Reaction Engineering - CSTR 2>re2.c_T - Concentration - mol/m³**.

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

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

5 In the table, enter the following settings:

Legends
Ideal tank 1
Ideal tank 2

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

The third plot group will not be used and can be deleted.

Concentration (re2)

In the **Model Builder** window, right-click **Concentration (re2)** and choose **Delete**.

Add a new study node for the optimization calculations.

ADD STUDY

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

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

3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies> Time Dependent**.

4 Click **Add Study** in the window toolbar.

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

STUDY 2

Step 1: Time Dependent

1 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.

2 In the **Output times** text field, type 24000.

Add an **Optimization** study step to perform the parameter estimation calculations.

3 In the **Model Builder** window, click **Study 2**.

4 In the **Settings** window for **Study**, type Study 2: Parameter estimation in the **Label** text field.

Optimization

1 In the **Study** toolbar, click **Optimization**.

Select to use the Levenberg-Marquardt optimization method. This method is very efficient for this type of optimization; when no mesh is effected and no additional constraints are present.

2 In the **Settings** window for **Optimization**, locate the **Optimization Solver** section.

3 From the **Method** list, choose **Levenberg-Marquardt**.

The existing plots will be reused. Disable the generation of default plots.

4 In the **Model Builder** window, click **Study 2: Parameter estimation**.

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

6 Clear the **Generate default plots** check box.

Solution 2 (sol2)

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

2 In the **Settings** window for **Solution**, click **Compute**.

RESULTS

Simulation, Parameter estimation

1 In the **Model Builder** window, right-click **Simulation, Initial guess** and choose **Duplicate**.

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

3 Locate the **Data** section. From the **Dataset** list, choose **Study 2: Parameter estimation/ Solution 2 (sol2)**.

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

Legends
`Simulation, Parameter estimation`

5 In the **Concentration in Real Reactor** toolbar, click **Plot**.

Concentrations in CSTRs

1 In the **Model Builder** window, click **Concentrations in CSTRs**.

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

3 From the **Dataset** list, choose **Study 2: Parameter estimation/Solution 2 (sol2)**.

4 In the **Concentrations in CSTRs** toolbar, click **Plot**.

Display the estimated parameters in a table.

Global Evaluation 1

1 In the **Results** toolbar, click **Global Evaluation**.

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

3 From the **Dataset** list, choose **Study 2: Parameter estimation/Solution 2 (sol2)**.

4 From the **Time selection** list, choose **Last**.

5 Click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - CSTR 1>alpha - Global control variable alpha**.

6 Click **Add Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)>Reaction Engineering - CSTR 1>beta - Global control variable beta**.

7 Click **Evaluate**.