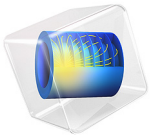

Parameter Estimation for Nonideal Reactor Models

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 optimizing the model results to experimental tracer data. Applying the **Global Least-Squares Objective** feature from the **Parameter Estimation** submenu makes this an easy task.

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

Note: This application requires the Chemical Reaction Engineering Module.

Model Definition

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

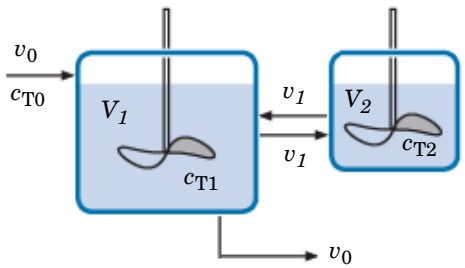

Figure 1: A real reactor can be modeled by two ideal CSTRs with interchange.

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

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.

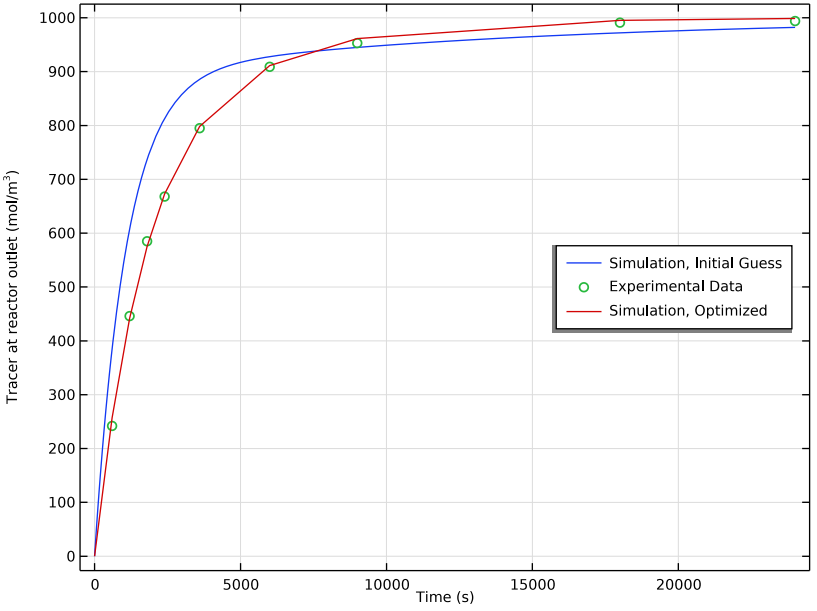

Figure 2: Model results and experimental data of the tracer concentration in the real reactor outlet.

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 **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 `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 **Name** section.

3 In the text field, type `T`.

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

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

2 In the text field, type `H2O`.

3 Locate the **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 **Chemical Formula** 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 **Chemical Formula** section.

3 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**.

COMPONENT 1 (COMP1)

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

REACTION ENGINEERING - CSTR 2

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

2 In the **Model Builder** window, under **Component 1 (comp1)** click **Reaction Engineering - CSTR 1.1 (re2)**.

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**.

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`.

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

RESULTS

Concentration in Non-Ideal Reactor

Now look at, and modify, the two default plot groups that were created.

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

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

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

4 Select the **y-axis label** check box. In the associated text field, type `Tracer at reactor outlet (mol/m<sup>3</sup>)`.

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

Simulation, Initial Guess

1 In the **Model Builder** window, expand the **Concentration in Non-Ideal Reactor** node, then click **Global 1**.

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

3 Click to expand the **Legends** section. Find the **Include** subsection. Select the **Label** check box.

4 Clear the **Solution** check box.

5 Clear the **Expression** check box.

6 In the **Concentration in Non-Ideal Reactor** toolbar, click **Plot**.

To plot the experimental data, add a **Table** and then a **Table Graph** to the plot group.

Experimental Data

1 In the **Results** toolbar, click **Table**.

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

3 Locate the **Data** section. Click **Import**.

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

Experimental Data

1 In the **Model Builder** window, right-click **Concentration in Non-Ideal Reactor** and choose **Table Graph**.

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

3 Click to expand the **Legends** section. Select the **Show legends** check box.

4 Find the **Include** subsection. Select the **Label** check box.

5 Clear the **Headers** check box.

6 In the **Concentration in Non-Ideal Reactor** toolbar, click **Plot**.

7 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **None**.

8 Find the **Line markers** subsection. From the **Marker** list, choose **Circle**.

Now look at the other default plot group.

Concentration in CSTRs

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

2 In the **Settings** window for **1D Plot Group**, type `Concentration in CSTRs` 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 **Middle right**.

Ideal CSTR 2

1 In the **Model Builder** window, expand the **Concentration in CSTRs** node, then click **Global 1**.

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

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

4 Right-click **Ideal CSTR 2** and choose **Duplicate**.

Ideal CSTR 1

1 In the **Model Builder** window, under **Results>Concentration in CSTRs** click **Ideal CSTR 2.1**.

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

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

Expression	Unit	Description
`re1.c_T`	`mol/m^3`	`Concentration`

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

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

COMPONENT 1 (COMP1)

Global Least-Squares Objective 1

1 In the **Model Builder** window, right-click **Component 1 (comp1)** and choose **Global Least-Squares Objective**.

Use the experimental data in the **Table** already created.

2 In the **Settings** window for **Global Least-Squares Objective**, locate the **Experimental Data** section.

3 From the **Data source** list, choose **Result table**.

4 Locate the **Data Column Settings** section. In the **Model expression** text field, type `re1.c_T`.

5 In the **Variable name** text field, type `c_T`.

6 In the **Unit** text field, type `mol/m^3`.

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 a **Parameter Estimation** 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.

Parameter Estimation

1 In the **Study** toolbar, click **Optimization** and choose **Parameter Estimation**.

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

3 Click **Add** twice.

4 In the table, enter the following settings:

Parameter name	Initial value	Scale	Lower bound	Upper bound
alpha (Volume fraction well stirred: To be estimated)	`0.5`	`0.5`	0	1
beta (Fluid exchange ratio: To be estimated)	`0.1`	`0.1`	0	1

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

5 Locate the **Parameter Estimation Method** section. From the **Method** list, choose **Levenberg-Marquardt**.

6 Click to expand the **Output While Solving** section. Before computing the optimization study, we want to choose to plot while solving. This makes it possible to visualize the optimization progress during computation.

7 In the **Model Builder** window, click **Parameter Estimation**.

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

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

10 In the **Study** toolbar, click **Get Initial Value**.

RESULTS

Simulation, Optimized

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

2 In the **Settings** window for **Global**, type `Simulation, Optimized` 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 **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
`re1.c_T`	`mol/m^3`	`Concentration`

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.

Now we can use the prepared plot to inspect the progress of the optimization.

STUDY 2: PARAMETER ESTIMATION

Parameter Estimation

1 In the **Model Builder** window, under **Study 2: Parameter Estimation** click **Parameter Estimation**.

2 In the **Settings** window for **Parameter Estimation**, locate the **Output While Solving** section.

3 Select the **Plot** check box.

4 From the **Plot group** list, choose **Concentration in Non-Ideal Reactor**.

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

RESULTS

Concentration in Non-Ideal Reactor

1 In the **Model Builder** window, under **Results** click **Concentration in Non-Ideal Reactor**.

2 In the **Concentration in Non-Ideal Reactor** toolbar, click **Plot**.

The estimated parameters, together with the values for the objective function, can be found in the Objective Probe Table 2.

Calculate the difference (root mean square) between the two simulations and the experimental data.

Comparison 1

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

2 In the **Settings** window for **Comparison**, locate the **Comparison** section.

3 From the **Metric** list, choose **RMS**.

4 In the **Concentration in Non-Ideal Reactor** toolbar, click **Plot**.

Comparison 1

1 In the **Model Builder** window, right-click **Simulation, Optimized** and choose **Comparison**.

2 In the **Settings** window for **Comparison**, locate the **Comparison** section.

3 From the **Metric** list, choose **RMS**.

4 In the **Concentration in Non-Ideal Reactor** toolbar, click **Plot**.