Solutions for Tutorial 6
Empirical Modelling

In this tutorial, you are going to apply the principles you have learned in Chapter 6 to identify a model of a chemical process empirically. The non-isothermal CSTR shown in Figure 6.1 is considered in this problem.

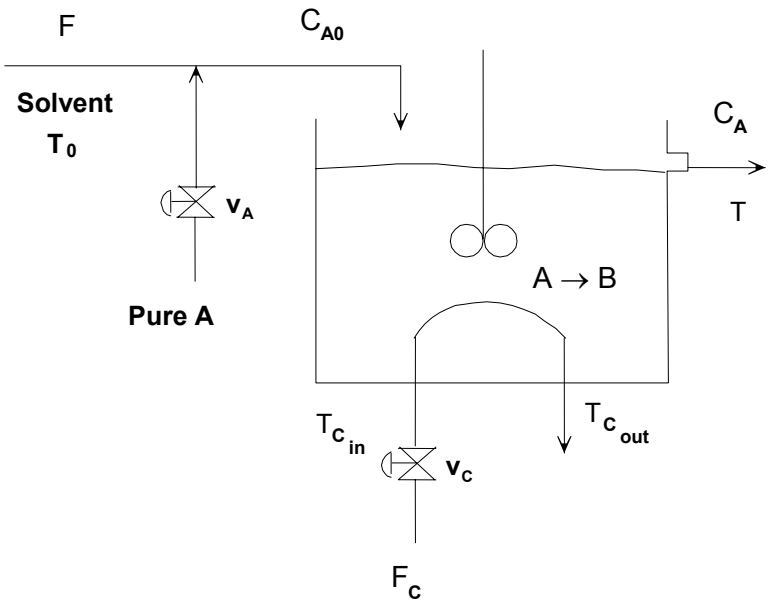

Figure 6.1 Non-isothermal CSTR with cooling coils.

Empirical Model Identification

An experiment has been performed to identify the model relating the reactor concentration, C_A, and the coolant valve opening, v_C. A step change of +20 % was introduced in v_C, and reactor concentration was measured using an analyzer. The process reaction curve is shown in Figure 6.2.

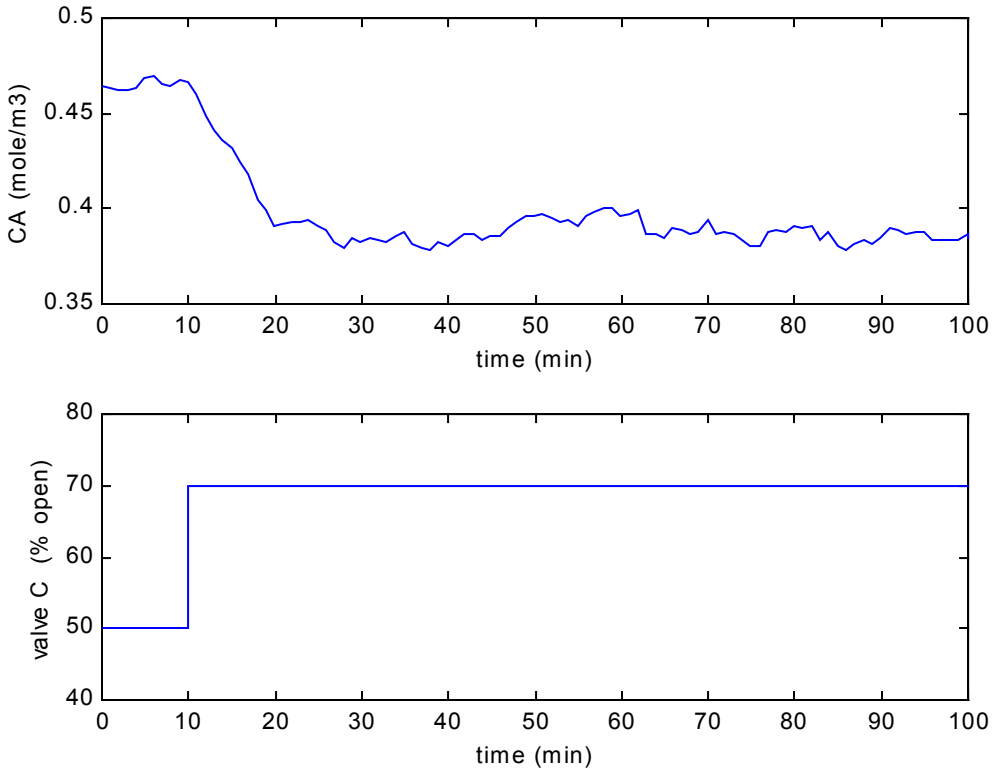

Figure 6.2 Process reaction curve for a step change in v_C.

6.1 Determine the parameters for the first order with dead time model.
6.2 Critique your results carefully.

Before we begin to perform the calculations, we must thoroughly evaluate the experiment and data to be sure that

1. the procedures were designed and performed correctly and
2. the data represents the process

Let's begin with the experiment procedures for the process reaction curve method.

Process reaction curve	True for this experiment?
Is the input signal nearly a perfect step?	**Yes**
Are the assumptions of output behavior valid? (i.e. smooth, S-shaped output response)	**Yes**
Did process begin at steady state?	**Yes**
Did the process achieve a new steady state?	**Yes**
Is the signal to noise ratio large enough?	**Yes**
Was the experiment repeated, process returned to initial operation	**No**

We see that the essential features have been satisfied. We can proceed with caution if the experiment has not been repeated.

Hint: Employ your understanding of the fundamental chemical engineering principles. Now, let's use our Chemical Engineering skills to evaluate the data.

- During the experiment, cooling valve c was opened by 20%.
- This should cool the reactor.
- Because of the temperature dependence of the reaction rate, the rate should decrease.
- Because the rate decreased, the concentration of reactant should increase in the reactor.

However, the experimental data indicate that the concentration **decreased**! Therefore, a severe inconsistency exists in the data. **We should not use the data**. We should repeat the experiment.

Many possible explanations are possible; just a few are given in the following.

- The feed temperature changed during the experiment.
- The feed concentration changed during the experiment.
- We plotted the % closed for valve c, but labeled it % open.

We must have data that conforms to the experimental methods and is consistent with chemical engineering principles before we build empirical models for process control.

Two additional experiments, +20% and –20% changes in v_C, were performed. The other input variables were monitored to make sure there were no changes. The process reaction curves for two different experiments are shown in Figure 5.3.

6.3 Discuss the good and poor aspects of these experiments for use with the process reaction curve modelling method.

Process reaction curve	True for this experiment?
Is the input signal nearly a perfect step?	**Yes**
Are the assumptions of output behavior valid? (i.e. smooth, S-shaped output response)	**Yes**
Did process begin at steady state?	**Yes**
Did the process achieve a new steady state?	**Yes**
Is the signal to noise ratio large enough?	**Yes**
Two steps to test for linearity	**Yes**
Agrees with engineering principles for chemical reactor	**Yes**
Was the experiment repeated, process returned to initial operation	**No**

Note that this data

- satisfies the essential experimental criteria, and
- is consistent with our qualitative understanding of the process dynamics.

We decide to use this data, given the careful monitoring of the process and two experiments, which allows checking of results.

6.4 Determine the parameters for the first order with dead time model using two different sets of experimental data.

For the step increase in the cooling valve opening:

$\delta = 20\%$

$\Delta =$ 0.084 mole/m^3 $\quad .63\Delta = 0.053$ mole/m^3 $\quad .28\Delta = 0.024$ mole/m^3

$t_{63\%} = 30$ min $\quad t_{28\%} = 14$ min

$K_p = \Delta/\delta = 0.0042$ [mole/m^3]/% open

$\tau = 1.5\ (t_{63\%} - t_{28\%}) = 24$ min

$\theta = t_{63\%} - \tau = 6$ min

For the step decrease in the cooling valve opening:

$\delta = -20\%$

$\Delta =$ 0.113 mole/m^3 $\quad .63\Delta = 0.71$ mole/m^3, $t_{63\%} = 23.3$ min $\quad .28\Delta = 0.032$ mole/m^3, $t_{28\%} = 12.8$ min

$K_p = \Delta/\delta = 0.0057$ [mole/m^3]/% open
$\tau = 1.5\ (t_{63\%} - t_{28\%}) = 15.8$ min
$\theta = t_{63\%} - \tau = 7.5$ min

The graphs are not large, so that errors in reading the distances can lead to different answers by different people. However, your answer should not be too different.

To check our calculations, you should plot the model on the same figure, so that the model can be compared with the experimental data. This will enable you to visually check the accuracy of the model.

6.5 Compare the parameter values in part c obtained from two different experiments, and explain any differences.

The model parameters are significantly different, compared with the likely errors introduced by the calculation procedure. However, the process is non-linear, and the changes in the valve opening are large compared with the maximum of ± 50% from its initial valve of 50% open. These differences are not unexpected.

A key question is, "Can we design a computer control approach for a system with dynamics that change with the magnitude in this example?"

We will see that the answer is **YES**, which makes the modelling effort worthwhile!

6.6 Discuss experimental designs that could help identify the problem encountered in question 6.1.

At a minimum, the experimental design should include a (second) step that returns the process to its original steady state. This gives a second set of data in the same operation. The models determined from the two experiments should be similar, within the errors introduced by sensor noise and graphical calculations.

If these models were very different, we would suspect a disturbance has occurred during the experiment, and we would repeat the procedure.

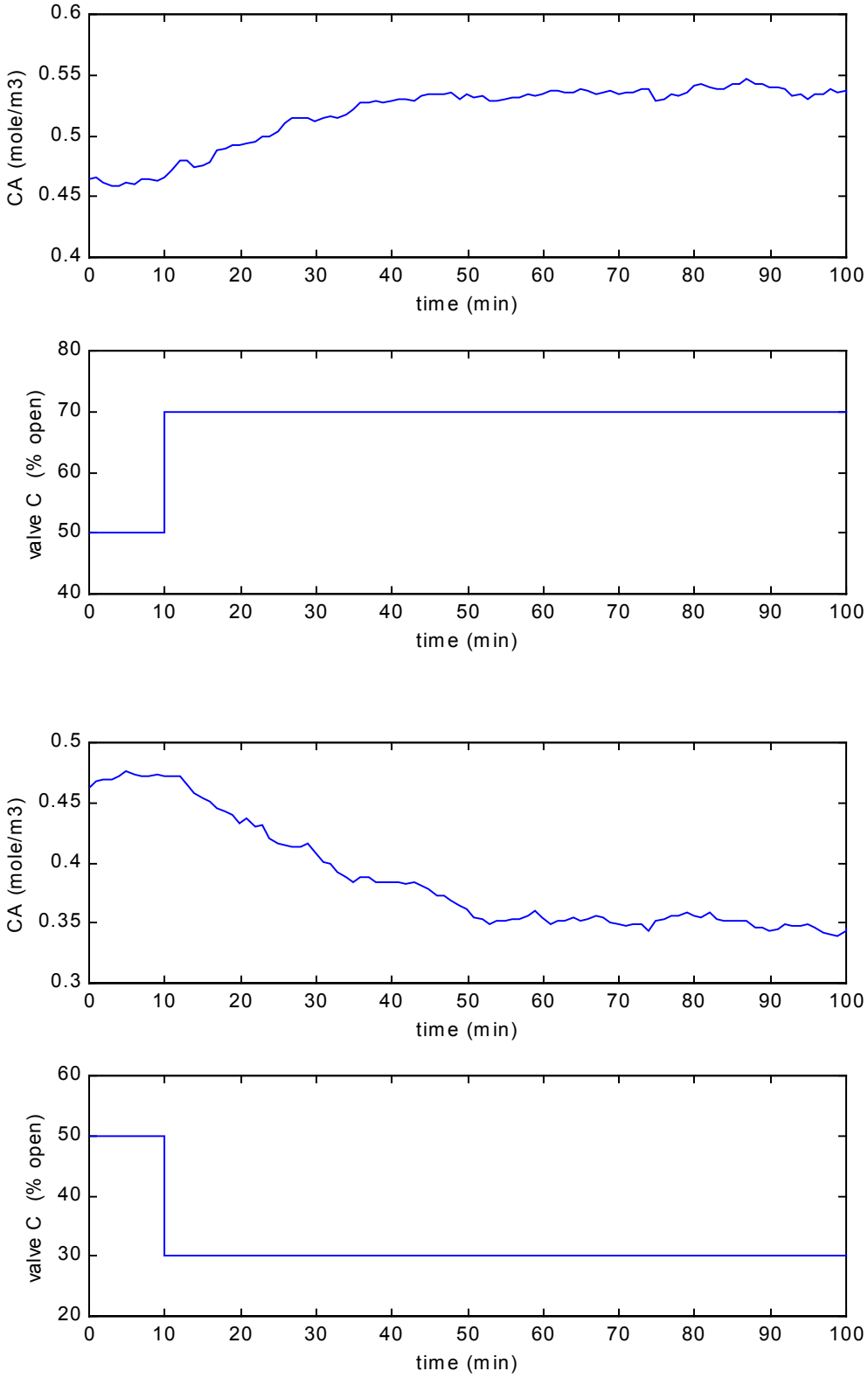

Figure 6.3. Process reaction curves for the CSTR without any unmeasured disturbances.

