CHAPTER 3

PROCESS DESCRIPTION

3.1 MATHEMATICAL MODEL OF CONTINUOUS STIRRED TANK REACTOR (CSTR)

A perfectly mixed Continuously Stirred Tank Reactor (CSTR) is shown in Figure 3.1. It is a single, first order exothermic irreversible reaction, \( A \rightarrow B \) in which a fluid stream is continuously fed to the reactor. Since the reactor is perfectly mixed the exit stream has the same concentration and temperature as the reactor fluid. The jacket surrounding the reactor also has feed and exit streams. The jacket is assumed to be perfectly mixed and at a lower temperature than the reactor. Energy then passes through the reactor walls into the jacket, removes the heat generated by reaction. There are many examples of this type of reactors in industries. The industrial reactors typically have more complicated kinetics, but the characteristic behaviour is similar.

3.1.1 Assumptions made

- Cooling Jacket can be directly manipulated so that the energy balance around the jacket is not required
- Perfect Mixing
- Constant volume, parameter values and physical properties
- Negligible shaft work
3.1.2 Material Balance Equation

The rate of accumulation of material in the reactor is equal to the difference between rate of material inflow and outflow.

\[
\frac{dv}{dt} = F_{in} \rho_{in} - F_{out} \rho
\] (3.1)

Assuming a constant amount of material in the reactor \( \frac{dv}{dt} = 0 \),

\[ F_{out} \rho = F_{in} \rho_{in} \] (3.2)

Also assume that the density remains constant, then

\[ F_{out} = F_{in} = F \] (3.3)

3.1.3 Balance on Component A

The balance on component A is

\[
\frac{dVc_A}{dt} = Fc_A - FC_A - rV
\] (3.4)

where, \( r \) is the rate of reaction per unit volume.
3.1.4 Energy Balance Equation

The energy balance is

\[
\frac{d(V_\rho c_\rho(T - T_{\text{ref}}))}{dt} = F_c (T_f - T_{\text{ref}}) - F_c (T - T_{\text{ref}}) \\
+ (- \Delta H) V_r - UA (T - T_i)
\]

where, \(T_{\text{ref}}\) represents an arbitrary reference temperature for enthalpy.

3.1.5 State Variable Form of Dynamic Equations

Equations (3.4) and (3.5) can be written in the following state variable form since \(dV/dt = 0\).

\[
f_1 (C_A, T) = \frac{dC_A}{dt} = \frac{F}{V} (C_{Af} - C_A) - r
\]

\[
f_2 (C_A, T) = \frac{dT}{dt} = \frac{F}{A} (T_f - T) + \left( \frac{-\Delta H}{\rho c_p} \right) r - \frac{UA}{V \rho c_p} (T - T_i)
\]

It is assumed that the volume is constant. The reaction rate per unit volume given by Arrhenius expression is

\[
r = k_o \exp \left( \frac{-\Delta E}{RT} \right) C_A
\]

where, the reaction is of first-order.

3.1.6 Steady-State Solution

The steady-state solution is obtained when \(\frac{dC_A}{dt} = 0\) and \(dT/dt = 0\), that is
To solve these two equations, all parameters and variables except for two \((C_A\) and \(T)\) must be specified. The only controlled variable is the temperature of reactant \(A\) in the outlet stream, which is varied by regulating the coolant flow rate. All process disturbances are generated by a first order autoregressive model. In addition, all measured variables are disrupted by Gaussian white noise with different variances.

Equations (3.9) and (3.10) can be represented as a function of coolant flow rate \((q_c)\) as,

\[
\frac{dC_A}{dt} = \frac{F}{V} (C_A - C_A) - k_0 C_A \exp \left( \frac{-E}{RT} \right) \tag{3.11}
\]

\[
\frac{dT}{dt} = \frac{F}{V} (T_0 - T) - \left( \frac{-\Delta H}{\rho C_p} \right) \frac{k_0 \exp \left( \frac{-E}{RT} \right)}{\rho C_p} + \frac{\rho C_p C}{\rho C_p v} \frac{q_c}{v \rho C_p}
\]

\[
\left( 1 - \exp \left( \frac{-H_A}{\rho C_p q_c} \right) \right) (T_0 - T) \tag{3.12}
\]

The linear state space model of the system is obtained by taking the Jacobian form of Equations (3.10) and (3.11)

\[
A = \begin{pmatrix}
\frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\
\frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2}
\end{pmatrix} = \begin{pmatrix}
\frac{-F}{V} & -K_S & -K'_S C_A \tag{3.13}
\end{pmatrix}
\]

where \(x_1\) and \(x_2\) are the state variables reactor concentration \((C_A)\) and reactor temperature \((T)\) and
\[ K_s = K_0 \exp \left( \frac{-F}{RT} \right) \]  
\[ k_s' = \frac{\partial k_s}{\partial T} = k_s \left[ \frac{E}{RT^2} \right] \exp \left( \frac{-E}{RT} \right) \]  
\[ B = \begin{pmatrix} \frac{\partial \ell_1}{\partial u_1} \\ \frac{\partial \ell_1}{\partial u_2} \\ \frac{\partial \ell_2}{\partial u_1} \\ \frac{\partial \ell_2}{\partial u_2} \end{pmatrix} = \begin{pmatrix} 0 \\ \frac{U_A}{V \rho C_p} \end{pmatrix} \]

where \( u_2 \) is the coolant flow rate, the state space representation is given as

\[
\dot{X} = \begin{bmatrix} \frac{-F}{V} - k_s \\ \frac{\Delta H}{\rho C_p} - \frac{F}{V} - \frac{\rho_c C_p q_c}{\rho C_p V} \left( 1 - \exp \left( \frac{-h A}{q_c \rho C_p} \right) \right) + \frac{\Delta H}{\rho C_p} \cdot k_s C_A \end{bmatrix} \begin{bmatrix} C_A \\ C_T \end{bmatrix} + \begin{bmatrix} \frac{\rho_c C_p}{\rho C_p V} \left( 1 - \exp \left( \frac{-h A}{q_c \rho C_p} \right) \right) \cdot (T_{co} - T) \end{bmatrix} \begin{bmatrix} q_c \end{bmatrix} \]
\[ Y = \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} C_A \\ C_T \end{bmatrix} \]

Substituting the values in the Table 3.1 in Equations (3.13) and (3.16) for the operating condition \( q_c \) and \( F \) taken as 100 l/min and discrete state space matrices obtained as

\[ A = \begin{pmatrix} -0.1241 & -0.00016 \\ 7.445 & -0.05892 \end{pmatrix} \] and \[ B = \begin{pmatrix} 0.003153 \\ -0.8198 \end{pmatrix} \]

\[ C = \begin{pmatrix} 0 & 1 \end{pmatrix} \]

\[ D = \begin{pmatrix} 0 & 0 \end{pmatrix} \]

The sampling time (Ts) considered as 1 second
3.1.7 Steady State Operating Data of CSTR

The steady state operating data of the CSTR used in simulation studies is given in Table 3.1.

Table 3.1 Steady state operating data of CSTR

<table>
<thead>
<tr>
<th>Process variable</th>
<th>Normal operating condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>Measured Product Concentration ( (C_A) )</td>
<td>0.08235 mol/L</td>
</tr>
<tr>
<td>Reactor Temperature ( (T) )</td>
<td>441.81 K</td>
</tr>
<tr>
<td>Volumetric Flow rate ( (F) )</td>
<td>100 L/min</td>
</tr>
<tr>
<td>Reactor Volume ( (V) )</td>
<td>100 L</td>
</tr>
<tr>
<td>Feed Concentration ( (C_{Af}) )</td>
<td>1 mol/L</td>
</tr>
<tr>
<td>Feed Temperature ( (T_f) )</td>
<td>350 K</td>
</tr>
<tr>
<td>Coolant Temperature ( (T_{co}) )</td>
<td>350 K</td>
</tr>
<tr>
<td>Coolant Flow rate ( (q_c) )</td>
<td>100 L/min</td>
</tr>
<tr>
<td>Heat of Reaction ( (\Delta H) )</td>
<td>2e5 cal/mol</td>
</tr>
<tr>
<td>Reaction rate constant ( (k_0) )</td>
<td>7.2e10 (\text{min}^{-1})</td>
</tr>
<tr>
<td>Activation energy term ( (E/R) )</td>
<td>9980 K</td>
</tr>
<tr>
<td>Heat transfer term ( (UA) )</td>
<td>7e5 cal/(\text{min.K})</td>
</tr>
<tr>
<td>Liquid Density ( (\rho, \rho_c) )</td>
<td>1000 g/L</td>
</tr>
<tr>
<td>Specific Heat capacity ( (C_p, C_{pc}) )</td>
<td>1 cal/(g.K)</td>
</tr>
</tbody>
</table>

Figures 3.3 and 3.4 show the temperature and concentration responses of the CSTR for the coolant flow rate variation as shown in Figure 3.2. From the open loop response of the CSTR process shown in Figures 3.3 and 3.4, it can be concluded that the dynamic behaviour of the CSTR process is not the same at different operating points and the process is indeed non-linear.
3.2 MATHEMATICAL MODEL OF TWO TANK INTERACTING SYSTEM

The system shown in Figure 3.5 consists of two interacting tanks connected to each other through circular connecting pipes of circular cross section provided with a valve. The valves 1 and 2 introduce nonlinearity in
the system. For the dynamic model, the incoming mass flows $F_{in1}$ and $F_{in2}$ are defined as inputs, while the two measurements $h_1(t)$ and $h_2(t)$ (the height of fluid in tank) are considered as outputs. The dynamic model is derived using the incoming and outgoing mass flows and is described by the differential equations (3.19) and (3.20).

For Tank 1,

$$- = f_1$$  \hspace{1cm} (3.19)

For Tank 2,

$$- = f_2$$  \hspace{1cm} (3.20)

where the valve coefficients of tank 1 and tank 2 are $b_1 = s_1 a_1$ and $b_2 = s_2 a_2$.

![Diagram of Two Tank Interacting System](image)

**Figure 3.5 Two Tank Interacting System**

The physical parameters of the two tank process are given in Table 3.2.
Table 3.2 Physical parameters of two tank interacting process

<table>
<thead>
<tr>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Area of the tanks ($A_1, A_2$)</td>
<td>0.0154 m$^2$</td>
</tr>
<tr>
<td>Acceleration due to gravity (g)</td>
<td>9.81 m/sec$^2$</td>
</tr>
<tr>
<td>Maximum permissible height of water levels ($h_{\text{max}}$)</td>
<td>0.63 m</td>
</tr>
<tr>
<td>Cross section of the connecting pipes ($a_1$ and $a_2$)</td>
<td>0.005 m$^2$</td>
</tr>
<tr>
<td>Co-efficient of the connecting pipes ($s_1$ and $s_2$)</td>
<td>0.45</td>
</tr>
<tr>
<td>Nominal operating conditions</td>
<td></td>
</tr>
<tr>
<td>$h_1 = 0.4$ m</td>
<td></td>
</tr>
<tr>
<td>$h_2 = 0.3$ m</td>
<td></td>
</tr>
</tbody>
</table>

The nonlinear equations are linearized using the Jacobian matrices to get the ABCD parameters. The matrices are given below:

$$A = \begin{bmatrix} \frac{\partial f_1}{\partial h_1} & \frac{\partial f_1}{\partial h_2} \\ \frac{\partial f_2}{\partial h_1} & \frac{\partial f_2}{\partial h_2} \end{bmatrix} = \frac{-b_1}{2A_1\sqrt{h_1-h_2}} \quad \frac{-b_1}{2A_1\sqrt{h_1-h_2}} \quad \frac{b_1}{2A_1\sqrt{h_1-h_2}} \quad \frac{b_1}{2A_2\sqrt{h_1-h_2}} \quad \frac{b_2}{2A_2\sqrt{h_1-h_2}}$$  \hspace{1cm} (3.21)

$$B = \begin{bmatrix} \frac{\partial f_1}{\partial q_1} & \frac{\partial f_1}{\partial q_2} \\ \frac{\partial f_2}{\partial q_1} & \frac{\partial f_2}{\partial q_2} \end{bmatrix} = \begin{bmatrix} \frac{1}{\lambda_1} & 0 \\ 0 & \frac{1}{\lambda_2} \end{bmatrix}$$  \hspace{1cm} (3.22)

$$C = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}$$  \hspace{1cm} (3.23)

$$D = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}$$  \hspace{1cm} (3.24)

where $f_1$ and $f_2$ are the differential equations respectively. $q_1$ and $q_2$ are the inflow rates. On substituting the values given in Table 3.2 in the above set of equations and simplifying, the discrete matrices are obtained as
\[ A = \begin{bmatrix} 0.9071 & 0.0901 \\ 0.0901 & 0.8551 \end{bmatrix}; \quad B = \begin{bmatrix} 6.1817 & 0.3056 \\ 0.3056 & 6.0052 \end{bmatrix} \]

The sampling time (Ts) considered as 0.1 second.

Figure 3.6 shows the open loop responses of the two tank interacting system for the inflow rates \( F_{\text{in1}} \) and \( F_{\text{in2}} \) is given in Table 3.2.

![Figure 3.6 Open loop response of two tank interacting system](image)

3.3 SYSTEM IDENTIFICATION REAL TIME PROCESS

3.3.1 Experimental Setup

This Research work was financially supported by the UGC Major Research Project scheme under the title of Investigations on the application of state estimation in continuous stirred tank reactor (CSTR) control and grant order No. F. 39-874/2010(SR) dated 12.01.2011
The P&I Diagram of CSTR bench mark system is shown in Figure 3.7

![Figure 3.7 P& I Diagram of CSTR Bench mark system](image)

A standalone Desktop PC was provided for Monitoring purpose. The hardware setup of the CSTR process and associated interface system are shown in the Figure 3.8 and Figure 3.9 respectively.

![Figure 3.8 Hardware setup of CSTR Process](image)
3.3.2 CSTR Specification Details

Storage Tank capacity: Appr. 125 Ltr.
Size: 500mm(L) X 500mm(W) X 500mm(H)

Heating and Circulation tank
Flow: 0 to 1400 LPH
Level: 0 to 500 mm
Inner Tank capacity: Appr. 70 Ltr
Size: Dia.350mm X 750mm(L)
Outer Tank capacity: Appr. 30 Ltr
Size: Dia.415mm X 800(L)

Single Phase Thyristor Power Controller
Voltage: Max.240V
Temperature: 27°C to 100°C
Current: Max.40A
Control Signal: 4-20MA & (1-5)V
Single Phase Heating Coil 3KW
I/P : Single Phase 230V, 50HZ, A/C supply
Process Line Size: 3/4”SS Pipe
3.3.3 Identification of CSTR- Temperature process model

System Identification is an approach to find a function that will map the input and output time series on to the parameter space such that some objective function $\in (y - \hat{y})$ is satisfied. The knowledge of the model is necessary for the design of soft sensing technique and model based control system. System identification is an experimental approach for determining the dynamic model of a system. It includes four steps:

1) Input/output data acquisition under an experimentation protocol
2) Selection or estimation of the “model” structure
3) Estimation of the model parameters
4) Validation of the identified model (structure and values of the parameters)

A complete identification operation must necessarily comprise the four stages indicated above. The specific methods used at each stage depend on the type of model desired (parametric or non-parametric, continuous-time or discrete-time) and on the experimental conditions (for example: hypothesis on the noise, open loop or closed loop identification).

The validation is the mandatory step to decide if the identified model is acceptable or not. As there does not exist a unique parameter estimation algorithm and a unique experimental protocol that always lead to a good identified model, the models obtained may not always pass the validation test. In this case, it is necessary to reconsider the estimation algorithms, the model complexity or the experimental conditions. System identification should be then considered as an iterative procedure as illustrated in Figure 3.10.
Figure 3.10  Flow diagram of System Identification

The inputs were feed water flow and coolant flow rate. The measured output variable is temperature of the reactor. The Input and output data were collected for the above real process using Compact RIO modules in real time. The average feed flow is maintained as constant value. The temperature data was collected till it reaches steady state. A step change was given in coolant flow rate and temperature was measured once again till it reaches steady state. All the values were obtained in terms of (1-5) Volts in order to normalize them within a single unit range and shown in Figure 3.11.

Figure 3.11 View of Sample Data Collection Using Compact RIO Modules

The parametric model approach was used for system identification. Recursive Least Square (RLS) (Ljung, 1999) method is used for estimating the
parameters. After the completion of parameter estimation, results were validated against a new set of data for same operating conditions. The Actual plant output vs. Identified Model response is shown in Figure 3.12.

Figure 3.12 Comparison of Open loop response of Actual plant and Identified Model

Thus the Mathematical model of CSTR real process was obtained in the form of discrete state space form and is shown here.

\[
X(k + 1) = \begin{bmatrix}
0.707895 & 2.77556E − 17 \\
1.66533E − 16 & 0.273895
\end{bmatrix} X(k) + \\
\begin{bmatrix}
0.00146101 & 0.354851 \\
0.000697335 & 0.3271436
\end{bmatrix} u(k)
\]

\[
Y(k) = [2.71197 \ 0.172458] X(k) + [0.00146101 \ 0.354851] u(k)
\]

where, U(k) :

- U₁(k) is Coolant flow (manipulated variable)
- U₂(k) is Feedwater Flow (treated as constant)
- Y(k) is Temperature (output variable)
3.3.4 Identification of Level process model

The same procedure is followed to identify the CSTR level process model also. The Experimental setup of level process and associated data acquisition system is shown in Figure 3.13.

![Experimental setup for CSTR Level process](image)

The input is in flow of feed water. The measured output variable is water level of the process tank. The Input and output data were collected for the above real process using Compact RIO modules in real time. The average feed flow is maintained as constant value. The level data was collected till it reaches steady state for every 1 second. All the values were obtained in terms of (1-5) Volts in order to normalize them within a single unit range. The parametric model approach was used for system identification. Recursive least square (RLS) method is used for estimating the parameters. After the completion of parameter estimation, results were validated against a new set of data for same operating conditions. The Actual plant output vs. Identified Model response is shown in Figure 3.14
Thus the Mathematical model of CSTR level process was obtained in the form of discrete state space form and is shown here.

Where, \( u(k) \) is feed water inflow (input variable)

\( Y(k) \) is level of tank (output variable).