R9.2.1 Adding a Controller to a CSTR

Figure R9.2-1 shows a generic diagram for the control of a chemical process. The controller will function to minimize or correct for any unexpected disturbances that may upset the process. A control system will measure one of the output variables that must be controlled, \( Y \) (e.g., temperature, concentration), and compare it to a desired value \( Y_{sp} \), called the set point. The difference, between the actual value, \( Y \), and the desired value, \( Y_{sp} \), is called the error signal, \( e \). That is,

\[
e = Y - Y_{sp}
\]  

(R9.2-1)

If the error signal is not equal to zero, a controller will make the appropriate changes in one of the system manipulated inputs, \( Z \) (e.g., flow rate, jacket temperature) to try to force the output variable, \( Y \), to return to its set point, \( Y_{sp} \).

For example, in the CSTR example 9-6, let’s pick the effluent temperature in the reactor to be the output variable to be controlled (i.e., \( Y = T \)). Then define \( Y_{sp} \) to be the desired effluent temperature from the reactor. If the desired temperature is \( T_{sp} = 180^\circ \text{C} \) and the actual temperature in the reactor for some reason rises to \( 200^\circ \text{C} \) (i.e., \( T = 200^\circ \text{C} \)), then the error, \( e \), would be

\[
e = T - T_{sp} = 200 - 180 = 20
\]

Because the error, \( e \), is nonzero, this will cause the controller to react to reduce the error, \( e \), to zero. The controller will send a signal that will manipulate one of the input variables, \( Z \), such as the entering temperature, \( T_0 \), coolant flow rate, \( m_C \), or jacket temperature, \( T_a \). For example, suppose that we choose the coolant flow rate, \( m_C \), as the manipulated variable to be changed; then the controller would increase \( m_C \) in an attempt to reduce \( Y \) (i.e., \( T \)) until it matches the set-point value \( Y_{sp} = T_{sp} = 180 \). A schematic of this process is shown in Figure R9.2-2. Here we see that a fluctuation (e.g., rise) in the inlet temperature acts as a disturbance causing the reactor temperature to rise above the set-point value, producing an error signal. The error signal is acted upon by the controller to open the valve to increase the coolant flow rate, causing the reactor temperature to decrease and return to its set-point value.
There are different types of controller actions that will make adjustments in the input, $Z$, based on the error between the output and set point. We shall consider five types: proportional, integral, derivative, proportional-integral, and proportional-integral-derivative actions.

- **Proportional action (P):** The adjustment of the manipulated input variable $Z$, is proportional to the error, $e = Y_{sp} - Y$:

  $Z = Z_0 + k_C e$  \hspace{1cm} (R9.2-2)

The parameter $Z_0$ is called the controller bias and is the value of the manipulated input at the time the controller is turned on. The proportionality constant $k_C$ is called the controller gain. The optimal value of $k_C$ depends on the process. With proportional action the manipulated variable will continue to change to correct the offset as long as the measured variable keeps changing. Once the measured variable stops changing, the manipulated variable will stop changing whether or not the measured variable is at its set point. Since this controller uses the value of the error to adjust the input to the process, this type of controller can never fully return the output variable to its set point. This is a disadvantage of proportional action. Proportional action is seldom used by itself as a means of controlling the process.

- **Integral action (I):** The adjustment of the input variable is proportional to the integral of the error, $e = Y - Y_{sp}$:

  $Z = Z_0 + \frac{k_C}{\tau_I} \int_0^t e \, dt$  \hspace{1cm} (R9.2-3)

The parameter $\tau_I$ is called the integral time constant. For a reactor it has the order of magnitude at the space time. Integral control action can also be expressed by the coupled set of equations

$$\frac{dI}{dt} = e$$

and
The optimal value of the proportionality constants, $k_C$ and $\tau_I$, are dependent on the process. With integral control the manipulated variables will continue to change to correct the upset as long as the integral of the error is nonzero. That is, the controller continues to manipulate the input variable until the error is zero. The main advantage of integral action is that over the long term the measured variable will always return to the set point. The disadvantage is that with this controller the response can become very oscillatory. Like proportional action, integral action is seldom used by itself.

- **Derivative action (D):** The rate of adjustment of the input variable is proportional to the time rate of change of the error (i.e., $de/dt$).

$$ Z = Z_0 + \frac{k_C}{\tau_D} \frac{de}{dt} $$  \hspace{1cm} (R9.2-5)

where $\tau_D$ is called the constant of proportionality for derivative action. The main problem with this type of action is that it can be very sensitive to noise and the error is normally filtered before entering the controller. Like proportional and integral action, derivative action is seldom used by itself.

- **Proportional-integral actions (PI):** The adjustment of the input variable is accomplished using both a proportional action and an integral action.

$$ Z = Z_0 + k_C e + \frac{k_C}{\tau_I} \int_0^t e \, dt $$  \hspace{1cm} (R9.2-6)

The advantage of this controller is that it has quick response for large errors and does not have set-point offset. The measured variable can be returned to the set point without excessive oscillation. Methods to tune your controller for the best value $\tau_I$, are discussed in Seborg, Edgar, and Mellichamp. In addition, you can use the Polymath on the CD-ROM supplied with this book to vary these parameters in Example Problems R9.2-1 and R9.2-2 to learn their effects.

- **Proportional-integral-derivative actions (PID):** The adjustment of the input variable is accomplished using all three methods—proportional, integral, and derivative—as follows:

$$ Z = Z_0 + k_C \left( e + \frac{1}{\tau_I} \int_0^t e \, dt + \tau_D \frac{de}{dt} \right) $$  \hspace{1cm} (R9.2-7)

The advantage of PID action is that it gives rapid response. The disadvantage is that you have to tune three parameters.

---

Now let’s apply the preceding discussion to control the exit temperature of a CSTR. The manipulated variable, $Z$, that will be used to control the temperature will be the coolant flow rate, $\dot{m}_C$, through the internal heat exchanger. A schematic diagram of this process is shown in Figure R9.2-3. To illustrate the response to a controller, we shall chose a controller with integral action to manipulate the coolant rate. For an integral action, the controller would activate the valve to change the flow rate using the following set of equations:

\[ \dot{m}_C = \dot{m}_{C_0} + \frac{kC}{\tau_I} I \]  \hspace{1cm} (R9.2-8)

\[ \frac{dI}{dt} = T - T_{sp} \]  \hspace{1cm} (R9.2-9)

The value $\dot{m}_{C_0}$ is the coolant rate at the time the controller is turned on.

**Figure R9.2-3** Control of a chemical reactor.

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**Example PRS.E9B–1 Integral Control if a CSTR**

We now reconsider Example 9-6 where a drop in the inlet temperature caused the reactor to operate at the lower steady state. However, we will now add an integral controller to the reaction system to learn what happens when the inlet temperature drops from 75°F to 70°F. The initial conditions at the time of the inlet temperature change are $C_A = 0.03789$, $C_B = 2.12$, $C_C = 0.143$, $C_M = 0.2266$ (all in lb mole/ft³), and $T = 138.5°F$. 

Sec. R9.2.1 Adding a Controller to a CSTR

Solution

For integral control we need to add two equations to our algorithm to obtain a relation between \( T \) and \( m_C \). For the CSTR reactor system at hand \( Z = m_c_0, Y = T \) and Equations (R9.2-3) and (R9.2-4) become

\[
\frac{dI}{dt} = T - T_{sp} \quad \text{(RE9-1.1)}
\]

\[
\dot{m}_C = \dot{m}_{CO} + \frac{k_C}{\tau_I} (I) \quad \text{(RE9-1.2)}
\]

The adjustment to be made to the coolant rate is calculated from the integral of the error, \( e \). The value of the proportionality constants, \( \tau_I \) and \( k_C \), are chosen to maximize performance of the system without sacrificing stability. The coolant rate will need to increase in order to decrease the outlet temperature \( T \) and vice versa. In this example we will choose the controller gain as \( k_C = 8.5 \) and the integral time \( \tau_I = V/l_{v_0} = 0.165 \) h. Methods of obtaining the best values of \( k_C \) and \( \tau_I \) can be found in textbooks on chemical process control. Equations (RE9-1.1) and (RE9-1.2) are added to the POLYMATH to represent an integral controller along with the initial conditions. (Note that all equations are the same as in Examples 9-5 and 9-6 other than the perturbed variable, \( T_0 \), and the variable being controlled, which is the coolant rate, \( m_C \).) Figure RE9-1.1 shows the reactor temperature as a function of time after the inlet temperature dropped to 70°F. The phase plane of reaction temperature and concentration is shown in Figure RE9-1.2 as they return to their original values after the change in inlet temperature. See Problem P9-2(j) for further analysis of this example.

![Figure RE9-1](image-url)  

Temperature-time trajectory.
Repeat Example RE9-1 using a proportional-integral controller instead of only an integral controller.

Solution

We note that while the output temperature returns to 138°F, the temperature oscillates over a 20°F range, which may be unacceptable in many situations. To overcome this we will add proportional to integral control. The equations here to be added to those in Table E9-4.1 (see the CD-ROM) to represent the PI controller are

\[
\frac{dI}{dt} = T - T_{sp} \quad \text{(RE9-2.1)}
\]

\[
m_c = m_{C0} + \frac{k_c}{\tau_i} (I) + k_c (T - T_{sp}) \quad \text{(RE9-2.2)}
\]

(Note that all equations are the same as before other than the perturbation variable and the variable being controlled.)

We will set \( k_c = 8.5 \) and \( \tau_i = \tau_p = 0.165 \) h. We see that the output outlet temperature does not oscillate as much as with just an integral controller. You can use the Polymath to try different controllers (differential, proportional, integral) and combinations thereof, along with different parameter values to study the behavior of CSTRs which have upsets to their system. Try \( k_c = 55 \) and \( \tau_i = 0.1 \).
### TABLE RE9.4-2.2. POLYMATH PROGRAM

<table>
<thead>
<tr>
<th>Equations:</th>
<th>Initial Values:</th>
</tr>
</thead>
<tbody>
<tr>
<td>d(Ca)/dt = 1/tau*(Ca0-Ca) + ra</td>
<td>0.03789</td>
</tr>
<tr>
<td>d(CB)/dt = 1/tau*(CB0-CB) + ra</td>
<td>0.12</td>
</tr>
<tr>
<td>d(Cc)/dt = 1/tau*(Cc0-Cc) - ra</td>
<td>0.143</td>
</tr>
<tr>
<td>d(Cm)/dt = 1/tau*(Cm0-Cm)</td>
<td>0.2255</td>
</tr>
<tr>
<td>d(r1)/dt = -(O-Fao<em>ThetaCp</em>(T1-10)+(36000)<em>ra</em>V)/4*cp</td>
<td>138.53</td>
</tr>
<tr>
<td>d(t1)/dt = T-Tap</td>
<td>0</td>
</tr>
</tbody>
</table>

Fao=600
T0=70
V=(1/7.484)*500
Tsp=135
UA=16000
Ta1=60
kC=6.5
k=16.9812*exp(-32400/1.967/(1+40))
Fb0=1000
Fm0=100
mc0=1000
rs=-k*Ca
NO=Cmmax*Kx1+Cmmax*Kx2*48+Cmmax*Kx19.5
ThetaCp=254+Fb0/Fao*ThetaFm0/Fm0*19.5
v0=Fmv0/0.923+Fb0/3.45+Fm0/1.54
Ca0=Fao/V0
Cb0=Fb0/V0
Cm0=Fm0/V0
Tm=V0/V0
X=(Ca0-Ca)/Ca0
m=mc0+Kc/tau1
T2a=-(T-Ta1)*exp(-UA/(18*mc))
Q=mc10*(Ta2-Ta1)
t0 = 0, tT = 4

Try different controllers (differential, proportional, integral) and combinations thereof, along with different parameter values to study the behavior of CSTRs that have upsets to their system (Figures RE9.4-2.1 and RE 9.4-2.2).
Figure RE9.4-2.1  Temperature-time trajectory.

Figure RE9.4-2.2  Conversion–temperature phase trajectory.