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CHAPTER 2

Plantwide Control Fundamentals

2.1 Introduction

In this chapter we examine some of the fundamental features and properties of the plantwide control problem. Our goal is to explain why we must design a control system from the viewpoint of the entire plant and not just combine the control schemes of each individual unit.

A typical chemical plant flowsheet has a mixture of multiple units connected both in series and in parallel. As noted in the previous chapter, the common topology consists of reaction sections and separation sections. Streams of fresh reactants enter the plant by being fed into the reaction section (or sometimes into the separation section) through a heat exchanger network. Here the chemical transformations occur to produce the desired species in one or more of a potentially wide array of reactor types: continuous stirred tank, tubular, packed bed, fluidized bed, sparged, slurry, trickle bed, etc.

The reactor effluent usually contains a mixture of reactants and products. It is fed into a separation section where the products are separated by some means from the reactants. Because of their economic value, reactants are recycled back to upstream units toward the reactor. The products are transported directly to customers, are fed into storage tanks, or are sent to other units for further processing. The separation section uses one or more of the fundamental unit operations: distillation, evaporation, filtration, crystallization, liquid-liquid extraction, adsorption, absorption, pressure-swing adsorption, etc. In this book we typically use distillation as the separation method because of its widespread use and our considerable experience with it. Everyone is a victim of his or her experience. Our backgrounds are in petroleum processing

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and chemical manufacturing, where distillation, despite frequently occurring predictions to the contrary, remains the premier separation method. However, the general principles also apply to processes with other separation units.

In addition to recycle streams returned back to upstream units, thermal integration is also frequently done. Energy integration can link units together in locations anywhere in the flowsheet where the temperature levels permit heat transfer to occur. The reaction and separation sections are thus often intimately connected. If conditions are altered in the reaction section, the resulting changes in flowrates, compositions, and temperatures affect the separation section and vice versa.

Changes in temperatures and thermal conditions can propagate into the separation section and significantly degrade dynamic performance. Changes in flowrates create load disturbances that can be recycled around a material loop. Changes in stream compositions fed into the separation section are also troublesome disturbances because they alter separation requirements (the work of separation is often a strong function of the feed mixture composition). Significant shifts in the compositions and flowrates within the separation section are needed to achieve the desired purities of product and recycle streams. Achieving a composition change can sometimes take a long time because the component inventories within the separation section must be varied and this inherently governs the system's dynamic behavior.

So we must pay particular attention to the effects of the reaction section on the separation section. In this chapter we strip away all of the confusing factors associated with complex physical properties and phase equilibrium so that we can concentrate on the fundamental effects of flowsheet topology and reaction stoichiometry. Therefore, in the processes studied here, we use such simplifying assumptions as constant relative volatilities, equimolal overflow, and constant densities.

These "ideal" physical property assumptions may appear to represent an overly simplistic view of the problem. Our experience, however, is that we can often gain significant insight into the workings and interactions of processes with recycle streams by not confusing the picture with complexities such as azeotropes. Considering the complexities of a real chemical system is, of course, vital at some stage. But we attempt in this chapter to focus on the "forest" and not on the individual "trees."

For example, suppose there is a stream in the process that is a binary mixture of chemical components A and B. If these components obey ideal vapor-liquid equilibrium behavior, we can use a single distillation column to separate them. If they form an azeotrope, we may have to use a two-column separation scheme. If the azeotropic composition controllability

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changes significantly with pressure, we can use a two-column sequence with each column operating at different pressures. If the azeotrope is homogeneous and minimum boiling, the two fairly pure product streams can be produced as bottoms products from the two columns. So there are two columns in the nonideal case instead of one column in the ideal case. But the reaction section and the recycle streams really don't care if we have one column or two. The reactor sees the same types of disturbances coming from the separation section, perhaps with different dynamics but with similar steady-state effects. Since many of the important plantwide and recycle effects are really steady-state phenomena, the idealized single-column separation section yields results that are similar to those of the complex two-column separation section.

2.2 Integrated Processes

Three basic features of integrated chemical processes lie at the root of our need to consider the entire plant's control system: (1) the effect of material recycle, (2) the effect of energy integration, and (3) the need to account for chemical component inventories. If we did not have to worry about these issues, then we would not have to deal with a complex plantwide control problem. However, there are fundamental reasons why each of these exists in virtually all real processes.

2.2.1 Material recycle

Material is recycled for six basic and important reasons.

1. *Increase conversion:* For chemical processes involving reversible reactions, conversion of reactants to products is limited by thermodynamic equilibrium constraints. Therefore the reactor effluent by necessity contains both reactants and products. Separation and recycle of reactants are essential if the process is to be economically viable.
2. *Improve economics:* In most systems it is simply cheaper to build a reactor with incomplete conversion and recycle reactants than it is to reach the necessary conversion level in one reactor or several in series. The simple little process discussed in Sec. 2.6 illustrates this for a binary system with one reaction $A \rightarrow B$. A reactor followed by a stripping column with recycle is cheaper than one large reactor or three reactors in series.
3. *Improve yields:* In reaction systems such as $A \rightarrow B \rightarrow C$, where B is the desired product, the per-pass conversion of A must be kept low to avoid producing too much of the undesirable product C. Therefore

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the concentration of B is kept fairly low in the reactor and a large recycle of A is required.

4. *Provide thermal sink:* In adiabatic reactors and in reactors where cooling is difficult and exothermic heat effects are large, it is often necessary to feed excess material to the reactor (an excess of one reactant or a product) so that the reactor temperature increase will not be too large. High temperature can potentially create several unpleasant events: it can lead to thermal runaways, it can deactivate catalysts, it can cause undesirable side reactions, it can cause mechanical failure of equipment, etc. So the heat of reaction is absorbed by the sensible heat required to raise the temperature of the excess material in the stream flowing through the reactor.
5. *Prevent side reactions:* A large excess of one of the reactants is often used so that the concentration of the other reactant is kept low. If this limiting reactant is not kept in low concentration, it could react to produce undesirable products. Therefore the reactant that is in excess must be separated from the product components in the reactor effluent stream and recycled back to the reactor.
6. *Control properties:* In many polymerization reactors, conversion of monomer is limited to achieve the desired polymer properties. These include average molecular weight, molecular weight distribution, degree of branching, particle size, etc. Another reason for limiting conversion to polymer is to control the increase in viscosity that is typical of polymer solutions. This facilitates reactor agitation and heat removal and allows the material to be further processed.

2.2.2 Energy integration

The fundamental reason for the use of energy integration is to improve the thermodynamic efficiency of the process. This translates into a reduction in utility cost. For energy-intensive processes, the savings can be quite significant. We can illustrate the use and benefits of energy-integration by considering again the HDA process introduced in the previous chapter (Fig. 1.1). Here energy is required to heat up the reactants in the furnace and to provide boilup in the three distillation columns. Heat must be removed in the separator condenser and in the three column condensers. Heat is generated in the exothermic reactor that normally would be removed through the plant utility system. However, by using a feed/effluent heat exchanger we can recover some of that energy. This reduces the amount of fuel required in the furnace to heat up the reactants and the duty required to cool the reactor effluent stream.

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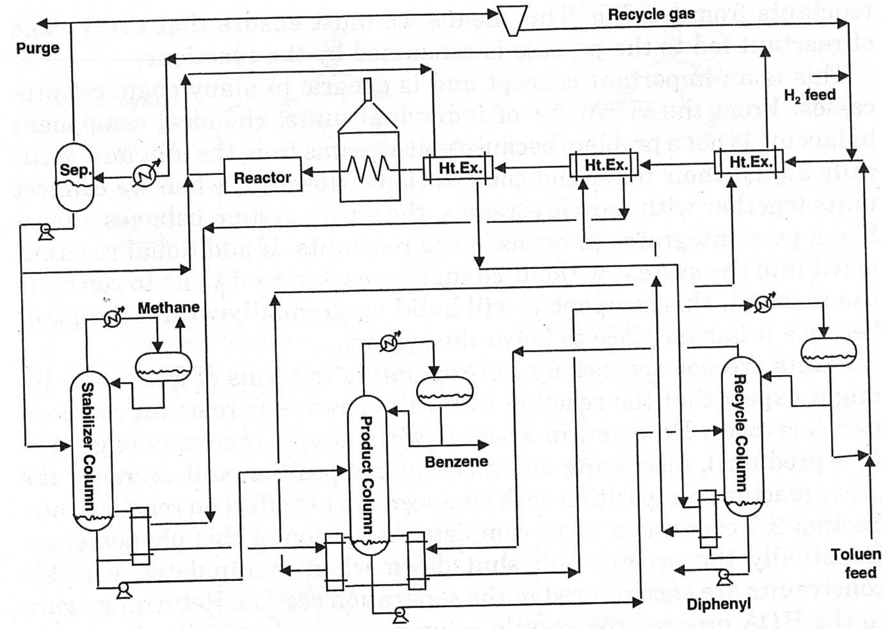

Figure 2.1 HDA process flowsheet with complex heat integration.

integration into the HDA process (Fig. 2.1). This is alternative 6 from the paper by Terrill and Douglas (1987). Heat from the reactor is used in reboilers of all three distillation columns. In addition, condensation of the overhead vapor from the recycle column provides heat input to the base of the product column. This is a good illustration of how units anywhere in the process can be linked together thermally. Figure 2.1 also shows how complex heat-integrated processes can quickly become, creating nontrivial control issues. This highlights why we cannot combine the control systems of individual unit operations in such processes.

2.2.3 Chemical component inventories

We can characterize a plant's chemical species into three types: reactants, products, and inerts. A material balance for each of these components must be satisfied. This is typically not a problem for products and inerts. However, the real problem usually arises when we consider reactants (because of recycle) and account for their inventories within the entire process. Every molecule of reactants fed into the plant must either be consumed via reaction or leave as an impurity or purge. Because of their value, we want to minimize the loss of reactants exiting the process since this represents a yield penalty. So we prevent

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reactants from leaving. This means we must ensure that every mole of reactant fed to the process is consumed by the reactions.

This is an important concept and is generic to many chemical processes. From the viewpoint of individual units, chemical component balancing is not a problem because exit streams from the unit automatically adjust their flows and compositions. However, when we connect units together with recycle streams, the entire system behaves almost like a pure integrator in terms of the reactants. If additional reactant is fed into the system without changing reactor conditions to consume the reactant, this component will build up gradually within the plant because it has no place to leave the system.

Plants are not necessarily self-regulating in terms of reactants. We might expect that the reaction rate will increase as reactant composition increases. However, in systems with several reactants (e.g., $A + B \rightarrow$ products), increasing one reactant composition will decrease the other reactant composition with an uncertain net effect on reaction rate. Section 2.7 contains a more complete discussion of this phenomenon. Eventually the process will shut down when manipulated variable constraints are encountered in the separation section. Returning again to the HDA process, the recycle column can easily handle changes in the amount of (reactant) toluene inventory within the column. However, unless we can somehow account for the toluene inventory within the entire process, we could feed more fresh toluene into the process than is consumed in the reactor and eventually fill up the system with toluene.

The three features outlined in this section have profound implications for a plant's control strategy. Simple examples in this chapter will illustrate the effects of material recycle and component balancing. Chapter 5 contains more details of the effects created by energy integration on the entire plant.

2.3 Units in Series

If process units are arranged in a purely series configuration, where the products of each unit feed downstream units and there is no recycle of material or energy, the plantwide control problem is greatly simplified. We do not have to worry about the issues discussed in the previous section and we can simply configure the control scheme on each individual unit operation to handle load disturbances.

If production rate is set at the front end of the process, each unit will only see load disturbances coming from its upstream neighbor. If the plant is set up for "on-demand" production, changes in throughput will propagate back through the process. So any individual unit will see load disturbances coming from both its downstream neighbor (flowrate changes to achieve different throughputs) and its upstream neighbor

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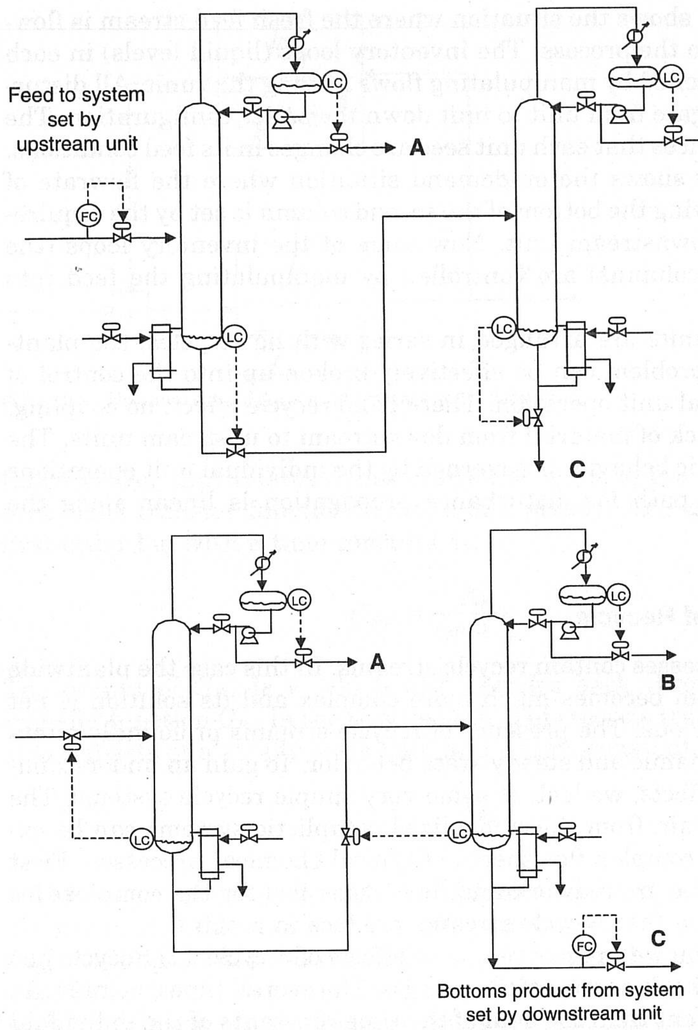

Figure 2.2 Units in series. (*a*) Level control in direction of flow; (*b*) level control in direction opposite flow.

(composition changes as the upstream units adjust to the load changes they see).

Figure 2.2 compares these two possible configurations for a simple plant. A fresh feed stream containing a mixture of chemical components A, B, and C is fed into a two-column distillation train. The relative volatilities are $\alpha_A > \alpha_B > \alpha_C$, and we select the "direct" (or "light-out-first") separation sequence: A is taken out the top of the first column and B out the top of the second column.

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Figure 2.2*a* shows the situation where the fresh feed stream is flow-controlled into the process. The inventory loops (liquid levels) in each unit are controlled by manipulating flows leaving that unit. All disturbances propagate from unit to unit down the series configuration. The only disturbances that each unit sees are changes in its feed conditions.

Figure 2.2*b* shows the on-demand situation where the flowrate of product *C* leaving the bottom of the second column is set by the requirements of a downstream unit. Now some of the inventory loops (the base of both columns) are controlled by manipulating the feed into each column.

When the units are arranged in series with no recycles, the plantwide control problem can be effectively broken up into the control of each individual unit operation. There is no recycle effect, no coupling, and no feedback of material from downstream to upstream units. The plant's dynamic behavior is governed by the individual unit operations and the only path for disturbance propagation is linear along the process.

2.4 Effects of Recycle

Most real processes contain recycle streams. In this case the plantwide control problem becomes much more complex and its solution is not intuitively obvious. The presence of recycle streams profoundly alters the plant's dynamic and steady-state behavior. To gain an understanding of these effects, we look at some very simple recycle systems. The insight we obtain from these idealized, simplistic systems can be extended to the complex flowsheets of typical chemical processes. First we must lay the groundwork and have some feel for the complexities and phenomena that recycle streams produce in a plant.

In this section we explore two basic effects of recycle: (1) Recycle has an impact on the dynamics of the process. The overall time constant can be much different than the sum of the time constants of the individual units. (2) Recycle leads to the "snowball" effect. This has two manifestations, one steady state and one dynamic. A small change in throughput or feed composition can lead to a large change in steady-state recycle stream flowrates. These disturbances can lead to even larger dynamic changes in flows, which propagate around the recycle loop. Both effects have implications for the inventory control of components.

2.4.1 Time constants in recycle systems

Figure 2.3 gives a block-diagram representation of a simple process with recycle. The input to the system is u. We can think of this input as a flowrate. It enters a unit in the forward path that has a transfer

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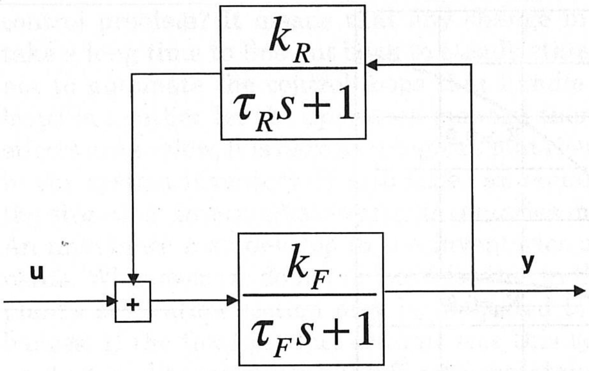

Figure 2.3 Simple block diagram of process with recycle.

function $G_{F(s)}$ that relates dynamically the input to the output of the unit. This transfer function consists of a steady-state gain K_F and a first-order lag with a time constant τ_F:

$$G_{F(s)} = \frac{K_F}{\tau_F s + 1} \tag{2.1}$$

The output of $G_{F(s)}$ is y, which also recycles back through a second transfer function $G_{R(s)}$ in the recycle path. This recycle transfer function also consists of a steady-state gain and a time constant.

$$G_{R(s)} = \frac{K_R}{\tau_R s + 1} \tag{2.2}$$

The output of the recycle block is added to the original input to the process u, and the sum of these two signals enters the forward block $G_{F(s)}$. It is important to note that the recycle loop in this process features *positive* feedback, not *negative* feedback that we are used to dealing with in feedback control. Most recycles produce this positive feedback behavior, which means that an increase in the recycle flowrate causes an increase in the flowrates through the process.

Some simple algebra gives the overall relationship for this system between input and output.

$$\frac{y_{(s)}}{u_{(s)}} = \frac{\dfrac{K_F}{\tau_F s + 1}}{1 - \left(\dfrac{K_F}{\tau_F s + 1}\right)\left(\dfrac{K_R}{\tau_R s + 1}\right)} = \frac{K_F(\tau_R s + 1)}{\tau_F \tau_R s^2 + (\tau_F + \tau_R)s + (1 - K_F K_R)} \tag{2.3}$$

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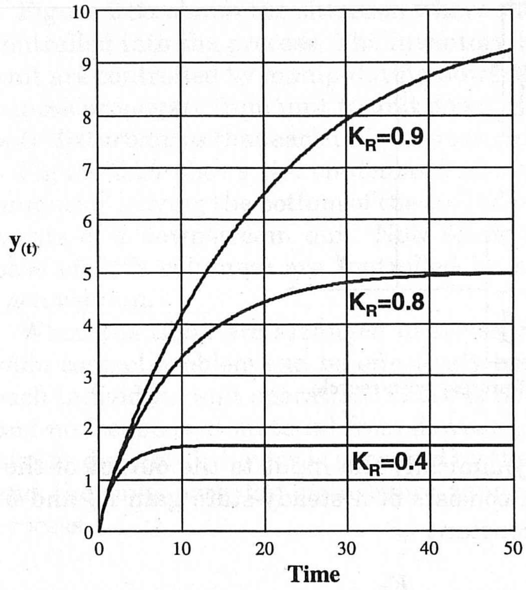

Figure 2.4 Effect of recycle loop gain on overall dynamic response.

The denominator of the transfer function is the characteristic equation of any system, so the characteristic equation of this recycle system is

$$\tau_F\tau_R s^2 + (\tau_F + \tau_R)s + (1 - K_F K_R) = 0 \tag{2.4}$$

$$\frac{\tau_F\tau_R}{(1 - K_F K_R)}\, s^2 + \frac{(\tau_F + \tau_R)}{(1 - K_F K_R)}\, s + 1 = 0 \tag{2.5}$$

This is the standard form of a second-order system, whose time constant is $\sqrt{\tau_F\tau_R/(1 - K_F K_R)}$. As the loop gain in the system $K_F K_R$ (the product of the gains in all units in the forward and recycle path) approaches unity, the time constant of the overall process becomes large. Hence the time constant of an entire process with recycle can be much larger than any of the time constants of its individual units. Figure 2.4 illustrates this for several values of $K_F K_R$. The value of K_F is constant at unity for these plots, as are the values of τ_F and τ_R. We can see that the effective time constant of the overall process is 25 minutes when $K_R = 0.9$, while the time constants of the individual units are equal to 1 minute. The steady-state gain of the process is $K_F/(1 - K_F K_R)$, so the steady-state effect of the recycle stream also becomes larger as the loop gain approaches unity.

What are the implications of this phenomenon for the plantwide

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control problem? It means that any change in a recycle process can take a long time to line out back to steady state. We are then tempted not to automate the control loops that handle inventories in recycle loops but rather let the operators manage them. Because the recycle effects are so slow, it is hard to recognize that there is a growing problem in the system inventory. It also takes an equally long time to rectify the situation. Intermediate vessel inventories may overfill or go empty. An imbalance may develop in the inventories of intermediate components. Whenever we do not account for this in the control strategy, the plant's separation section may be subjected to ramplike load disturbances. If the final product column sees this type of disturbance, the product quality controller has difficulty maintaining setpoint. To handle ramp disturbances, special low-frequency-compensated controllers can be used. But these types of controllers are not typically implemented either in conventional control or MPC systems (Belanger and Luyben, 1997). Morud and Skogestad (1996) present a more detailed analysis of the effect of material recycle and heat integration on the dynamic behavior of integrated plants.

2.4.2 Snowball effects

Another interesting observation that has been made about recycle systems is their tendency to exhibit large variations in the magnitude of the recycle flows. Plant operators report extended periods of operation when very small recycle flows occur. It is often difficult to turn the equipment down to such low flowrates. Then, during other periods when feed conditions are not very different, recycle flowrates increase drastically, usually over a considerable period of time. Often the equipment cannot handle such a large load.

We call this high sensitivity of the recycle flowrates to small disturbances the *snowball effect*. We illustrate its occurrence in the simple example below. It is important to note that this is *not* a dynamic effect; it is a *steady-state* phenomenon. But it does have dynamic implications for disturbance propagation and for inventory control. It has nothing to do with closed-loop stability. However, this does not imply that it is independent of the plant's control structure. On the contrary, the extent of the snowball effect is very strongly dependent upon the control structure used.

The large swings in recycle flowrates are undesirable in a plant because they can overload the capacity of the separation section or move the separation section into a flow region below its minimum turndown. Therefore it is important to select a plantwide control structure that avoids this effect. As the example below illustrates and as

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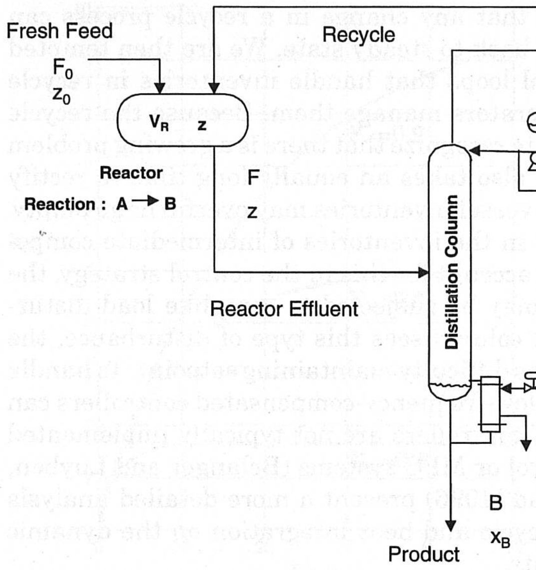

Figure 2.5 Flowsheet of binary recycle process.

more complex processes discussed in later chapters also show, a very effective way to prevent the snowball effect is to apply the following plantwide control heuristic:

> A stream somewhere in each liquid recycle loop should be flow controlled.

Luyben rule

Let us consider one of the simplest recycle processes imaginable: a continuous stirred tank reactor (CSTR) and a distillation column. As shown in Figure 2.5, a fresh reactant stream is fed into the reactor. Inside the reactor, a first-order isothermal irreversible reaction of component A to produce component B occurs $A \rightarrow B$. The specific reaction rate is k (h^{-1}) and the reactor holdup is V_R (moles). The fresh feed flowrate is F_0 (moles/h) and its composition is z_0 (mole fraction component A). The system is binary with only two components: reactant A and product B. The composition in the reactor is z (mole fraction A). Reactor effluent, with flowrate F (moles/h) is fed into a distillation column that separates unreacted A from product B.

The relative volatilities are such that A is more volatile than B, so the bottoms from the column is the product stream. Its flowrate is B (moles/h) and its composition is x_B (mole fraction A). The amount of A impurity in this product stream is an important control objective and must be maintained at some specified level to satisfy the product quality requirements of the customer.

The overhead distillate stream from the column contains almost all of component A that leaves the reactor because of the purity specifica-

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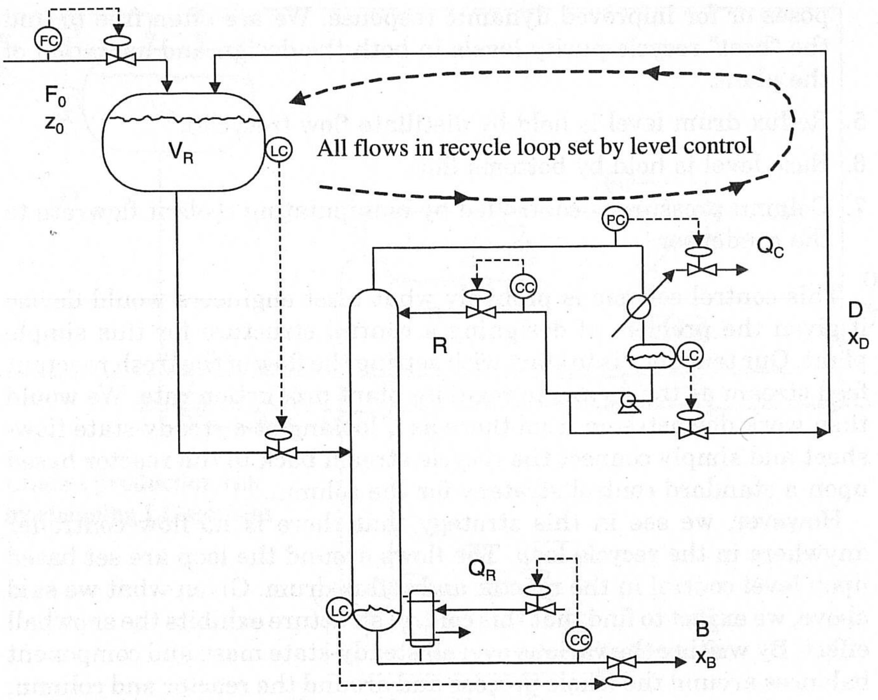

Figure 2.6 Conventional control structure with fixed reactor holdup.

tion on the bottoms stream. It is recycled back to the reactor at a flowrate D and with a composition x_D (mole fraction A). The column has N_T trays and the feed tray is N_F (counting from the bottom). The reflux flowrate is R and the vapor boilup is V (moles/h).

We now explore two alternative control structures for this process.

Conventional control structure. As shown in Fig. 2.6, the following control loops are chosen:

1. Fresh feed flow is controlled.
2. Reactor level is controlled by manipulating reactor effluent flow.
3. Bottoms product purity is controlled by manipulating heat input to the reboiler.
4. Distillate purity is controlled by manipulating reflux flow. Note that we have chosen to use dual composition control (controlling both distillate and bottoms purities) in the distillation column, but there is no *a priori* reason for holding the composition of the recycle stream constant since it does not leave the process. It may be useful to control the composition of this recycle stream for reactor yield pur-

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poses or for improved dynamic response. We are often free to find the "best" recycle purity levels in both the design and operation of the plant.

5. Reflux drum level is held by distillate flow (recycle).
6. Base level is held by bottoms flow.
7. Column pressure is controlled by manipulating coolant flowrate to the condenser.

This control scheme is probably what most engineers would devise if given the problem of designing a control structure for this simple plant. Our tendency is to start with setting the flow of the fresh reactant feed stream as the means to regulate plant production rate. We would then work downstream from there as if looking at a steady-state flowsheet and simply connect the recycle stream back to the reactor based upon a standard control strategy for the column.

However, we see in this strategy that there is no flow controller anywhere in the recycle loop. The flows around the loop are set based upon level control in the reactor and reflux drum. Given what we said above, we expect to find that this control structure exhibits the snowball effect. By writing the various overall steady-state mass and component balances around the whole process and around the reactor and column, we can calculate the flow of the recycle stream, at steady state, for any given fresh reactant feed flow and composition. The parameter values used in this specific numerical case are in Table 2.1.

With the control structure in Fig. 2.6 and the base-case fresh feed flow and composition, the recycle flowrate is normally 260.5 moles/h. However, the recycle flow must decrease to 205 moles/h when the fresh feed composition is 0.80 mole fraction *A*. It must increase to 330 moles/h when the fresh feed compositon changes to pure *A*. Thus a 25 percent change in the disturbance (fresh feed composition) results in a 60 percent change in recycle flow. With this same control structure and the base-case fresh reactant feed composition, the recycle flow drops to 187 moles/h if the fresh feed flow changes to 215 moles/h. It

TABLE 2.1 Process Data

Base-case fresh feed composition	0.9	mole fraction *A*
Base-case fresh feed flowrate	239.5	moles/h
Reactor holdup	1250	moles
Reactor effluent flowrate	500	moles/h
Recycle flowrate	260.5	moles/h
Specific reaction rate	0.34086	h^{-1}
Bottoms composition	0.0105	mole fraction *A*
Recycle composition	0.95	mole fraction *A*

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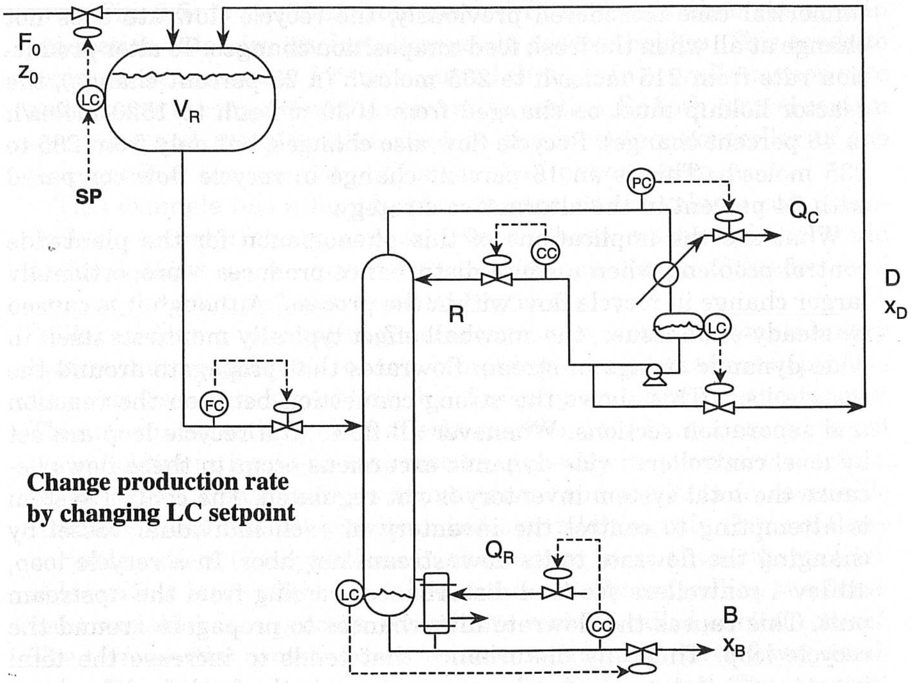

Figure 2.7 Control structure with variable reactor holdup.

must increase to 362 moles/h when the fresh feed flowrate is changed to 265 moles/h. Thus a 23 percent change in fresh feed flowrate results in a 94 percent change in recycle flowrate. These snowball effects are typical for many recycle systems when control structures such as that shown in Figure 2.6 are used and there is no flow controller somewhere in the recycle loop.

Variable reactor holdup structure. An alternative control structure is shown in Figure 2.7. This strategy differs from the previous one in two simple but important ways.

1. Reactor effluent flow is controlled.
2. Reactor holdup is controlled by manipulating the fresh reactant feed flowrate.

All other control loops are the same. We see here that we cannot change production rate directly by manipulating the fresh feed flow, because it is used to control reactor level. However, we must have some means to set plant throughput, which can be achieved indirectly in this scheme by changing the setpoint of the reactor level controller. Using the same numerical case considered previously, the recycle flowrate does not change at all when the fresh feed composition changes. To alter production rate from 215 moles/h to 265 moles/h (a 23 percent change), the reactor holdup must be changed from 1030 moles/h to 1520 moles/h (a 48 percent change). Recycle flow also changes, but only from 285 to 235 moles/h. This is an 18 percent change in recycle flow compared with 94 percent in the alternative strategy.

What are the implications of this phenomenon for the plantwide control problem, when a small disturbance produces a proportionally larger change in recycle flow within the process? Although it is caused by steady-state issues, the snowball effect typically manifests itself in wide dynamic swings in stream flowrates that propagate around the recycle loop. This shows the strong connection between the reaction and separation sections. Whenever all flows in a recycle loop are set by level controllers, wide dynamic excursions occur in these flows because the total system inventory is not regulated. The control system is attempting to control the inventory in each individual vessel by changing the flowrate to its downstream neighbor. In a recycle loop, all level controllers see load disturbances coming from the upstream unit. This causes the flowrate disturbances to propagate around the recycle loop. Thus any disturbance that tends to increase the total inventory in the process (such as an increase in the fresh feed flowrate) will produce large increases in all flowrates around the recycle loop.

2.5 Reaction/Separation Section Interaction

For the process considered in the previous section where the reaction is $A \rightarrow B$, the overall reaction rate depends upon reactor holdup, temperature (rate constant), and reactant composition (mole fraction A) $\mathcal{R} = V_R k z$. The two control structures considered above produce fundamentally different behavior in handling disturbances. In the first, the separation section must absorb almost all of the changes. For example, to increase production rate of component B by 20 percent, the overall reaction rate must increase by 20 percent. Since both reactor temperature (and therefore k) and reactor holdup V_R are held constant, reactor composition z must increase 20 percent. This translates into a very significant change in the composition of the feed stream to the separation section. This means the load on the separation section changes significantly, producing large variations in recycle flowrates.

In the second structure, *both* reactor holdup V_R and reactor composition z can change, so the separation section sees a smaller load disturbance. This reduces the magnitude of the resulting change in recycle flow because the effects of the disturbance can be distributed between the reaction and separation sections.

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Dynamic controllability

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ture (Fig. 2.6) is modified from normal PI to P only, then changes in production rate also produce changes in reactor holdup. This tends to compensate somewhat for the required changes in overall reaction rate and lessens the impact on the separation section. So both control system structure and the algorithm used in the inventory controller of the reactor affect the amount of this snowball phenomenon.

This example has a liquid-phase reactor, where volume can potentially be varied. If the reactor were vapor phase, reactor volume would be fixed. However, we now have an additional degree of freedom and can vary reactor pressure to affect reaction rate.

We can draw a very useful general conclusion from this simple binary system that is applicable to more complex processes: changes in production rate can be achieved only by changing conditions in the reactor. This means something that affects reaction rate in the reactor must vary: holdup in liquid-phase reactors, pressure in gas-phase reactors, temperature, concentrations of reactants (and products in reversible reactions), and catalyst activity or initiator addition rate. Some of these variables affect the conditions in the reactor more than others. Variables with a large effect are called *dominant*. By controlling the dominant variables in a process, we achieve what is called *partial control*. The term partial control arises because we typically have fewer available manipulators than variables we would like to control. The setpoints of the partial control loops are then manipulated to hold the important economic objectives in the desired ranges.

The plantwide control implication of this idea is that production rate changes should preferentially be achieved by modifying the setpoint of a partial control loop in the reaction section. This means that the separation section will not be significantly disturbed. Using the control structure in Fig. 2.6, changes in production rate require large changes in reactor composition, which disturb the column. Using the control structure shown in Fig. 2.7, changes in production rate are achieved by altering the setpoint of a controlled dominant variable, reactor holdup, with only small changes in reactor composition. This means that the column is not disturbed as much as with the alternative control scheme.

Hence a goal of the plantwide control strategy is to handle variability in production rate and in fresh reactant feed compositions while minimizing changes in the feed stream to the separation section. This may not be physically possible or economically feasible. But if it is, the separation section will perform better to accommodate these changes and to maintain product quality, which is one of the vital objectives for plant operation. Reactor temperature, pressure, catalyst/initiator activity, and holdup are preferred dominant variables to control compared to direct or indirect manipulation of the recycle flows, which of course affect the separation section.

NEI.

control structure that does not work

In Chaps. 4 and 6 we discuss specific control issues for chemical reactors and distillation columns. We shall then have much more to say about the important concepts of dominant variables and partial control. Much of the material in those chapters centers on the control of the units individually. However, we also try to show how plantwide control considerations may sometimes alter the control strategy for the unit from what we would normally have in an isolated system.

Some of our previous discussion provides selected clues about why the "best" control structure for an isolated reactor or column may not be the best control strategy when plantwide dynamics are considered.

Let's look again at the simple reactor/column process in Fig. 2.5. In Sec. 2.4.2 we proposed two control structures where both the bottoms composition x_B (the plant product) and the distillate composition x_D (the recycle stream) are controlled, i.e., dual composition control. Bottoms composition must be controlled because it is the product stream leaving the plant and sold to our customers. However, there is *a priori* no reason to control the composition of the recycle stream since this is an internal flow within the plant.

From the perspective of an isolated column, we can achieve better performance in bottoms product composition control by using simple single-end control. Dual composition control means two interacting control loops that normally must be detuned to achieve closed-loop stability. Single-end composition control means one SISO (single-input–single-output) loop that can be tuned up as tightly as the performance/robustness trade-off permits. If we look at just the operation of this distillation column with the control objective to do the best job we can to achieve on-aim product quality, then we would select a single-end control structure for the column.

However, our column is connected via material flow with a reactor. In Chap. 4 we show that reactor control often boils down to two issues: (1) managing energy (temperature control) and (2) keeping as constant as possible the composition and flowrate of the total reactor feed stream (fresh feed plus recycle streams). The latter goal implies that it may in fact be desirable to control the composition of the recycle stream. This minimizes the variablity in recycle impurity composition back into the reactor. This recycle composition is dictated by the economic trade-offs between yield, conversion, energy consumption in the separation section, and reactor size.

Our plantwide control perspective may push us to use a dual composition control system on the column. We would have to loosen up the bottoms composition loop tuning. But smoother reactor operation may reduce disturbances to the column and result in better product quality control.

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Dynamic
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These are the issues discussed in Part 2: the control of unit operations individually and as part of a plantwide flowsheet.

2.6 Binary System Example

Our simple process considered previously was arbitrarily specified to contain a flowsheet with a reactor, column, and recycle stream. If we step farther back and consider the design of this process, we have many alternative ways to accomplish our objective, which is to take a fresh feed stream containing mostly reactant A and convert it into a stream of mostly product B. In addition to the reactor/column/recycle configuration, we could accomplish the same task by using one large CSTR or by using several CSTRs in series. In this section we analyze these alternatives quantitatively by comparing their steady-state economics (that is, which flowsheet gives the minimum total annual cost considering capital plus energy cost). Then we discuss the dynamic controllability of these alternative flowsheets.

2.6.1 Steady-state design

We neglect the energy cost of cooling the reactor because this will be essentially the same for all alternative flowsheets. Therefore designs with only reactors have to consider just the capital cost of the reactor. Designs with a reactor and column have both energy costs (heat input to the reboiler) and capital costs (reactor, column, reboiler, condenser, and trays). We use here the installed capital costs correlations given by Douglas (1988). The cost of the reactor is assumed to be 5 times the cost of a plain tank. We use a payback period of 3 years to calculate the annual cost of capital.

$$\text{Annual capital cost} = \frac{\text{total capital cost}}{3} \tag{2.6}$$

Table 2.2 gives equipment sizes and cost data for several alternative designs. Molecular weights are assumed for simplicity to be 50 lb/mole and density is 50 lb/ft^3. An aspect ratio (diameter/length) of 0.5 is used.

TABLE 2.2 Economic Data for CSTRs

Number of CSTRs	1	2	3	4	5
Holdup per vessel, ft^3	59,523	5,802	2,395	1,435	1,009
Diameter, ft	33.6	15.5	11.5	9.7	8.63
Capital cost 10^6 \$	11.8	5.56	4.81	4.66	4.68
Annual capital cost, 10^6 \$/yr	3.95	1.86	1.60	$\boxed{1.55}$	1.56

output
that does not work

TABLE 2.3 Economic Data for CSTR and Stripper

Reactor size, ft^3	800	1000	2500	5000
Reactor diameter, ft	7.98	8.6	11.7	14.7
Trays in stripper	14	14	17	16
Recycle composition, mole fraction A	0.873	0.761	0.391	0.215
Column diameter, ft	8.24	6.04	3.71	3.21
Reboiler energy, 10^6 Btu/h	25.1	13.5	5.09	3.80
Area condenser, ft^2	8360	4496	1697	1267
Area reboiler, ft^2	5020	2698	1018	760
Capital cost, $1000:				
Reactor	810	1090	1645	2535
Column	304	218	152	124
Reboiler	396	264	140	116
Condenser	552	369	196	162
Trays	13	8	5	4
Total capital cost (10^6 $)	2.075	1.949	2.138	2.941
Annual costs, 10^6 $/yr:				
Energy	1.099	0.591	0.223	0.167
Capital	0.692	0.650	0.713	0.980
Total annual cost, 10^6 $/yr	1.79	1.24	$\boxed{0.936}$	1.15

Additional details of the economic and sizing calculations can be found in Luyben (1993). Notice that the flowsheet with the smallest annual cost has four CSTRs. Now let's compare this system with a process that has one CSTR and a column whose overhead product is recycled back to the reactor. Economic studies of this system have shown that a simple stripping column is cheaper than a full column. Table 2.3 gives size and cost data over a range of reactor sizes.

This simplistic economic evaluation shows that the reactor/stripper process is more economical than the reactors-in-series process. A 2500 ft^3 reactor followed by a stripping column can achieve the same result that would require four 1435 ft^3 reactors in series with no recycle.

In the simple binary process considered above, the 2500 ft^3 reactor with a 17-tray stripper gives the process with the smallest total annual cost: $936,000/yr versus $1,550,000/yr for the best of the CSTR-in-series flowsheets. Thus this process with recycle is more economical, from the viewpoint of steady state, than the alternative process consisting of reactors in series. This is the point we made in Sec. 2.2 about the economic advantage for recycle.

2.6.2 Dynamic controllability

Dynamic simulations of two alternative processes provide a quantitative comparison of their dynamic controllabilities. To strike a balance between simplicity and the economic optimum, we selected the three-CSTR process to compare with the reactor/stripper process. The scheme

Dynamic controllability

Inventory control

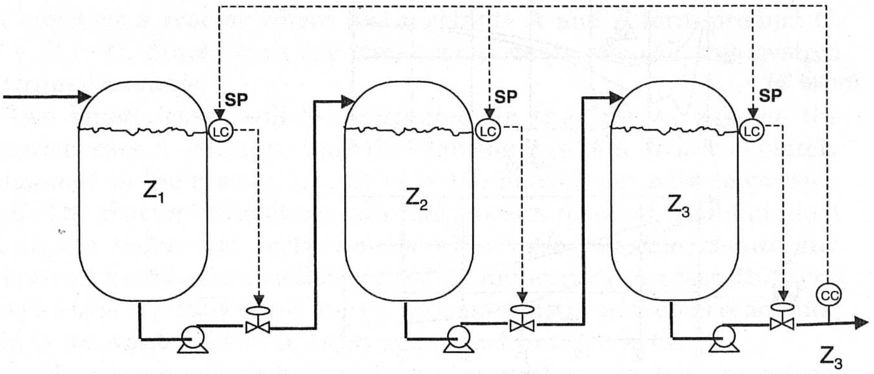

Figure 2.8 Three-CSTR control structure.

used for the three-CSTR process controls the composition of the final product leaving the third reactor (z_3) by changing the setpoint signal to three level controllers for the three vessels (Fig. 2.8). The composition controller has PI action with $K_c = 1$ and $\tau_I = 10.2$ min. A composition transmitter deadtime of 3 minutes is used. Fresh feed is flow-controlled. Level controllers are proportional-only with gains of 10.

The scheme for the reactor/stripper process uses a PI controller to hold product composition (x_B) by manipulating vapor boilup in the stripper. The same analyzer deadtime is used. Proportional level controllers are used for the stripper base (manipulating bottoms flow), the overhead receiver (manipulating recycle flow), and the reactor (manipulating reactor effluent flow) with gains of 2.

Figures 2.9 and 2.10 show the dynamic responses of the two alternative processes for step changes in the fresh feed composition z_0 and fresh feed flowrate F_0. Note the differences in the time scales. The three-CSTR process takes much longer to settle out after the disturbance occurs. However, the maximum deviation of product purity is about half that experienced with the reactor/stripper process. The large holdups in the three reactors filter the disturbances but also slow the process response.

Because the reactor/stripper process is much more attractive economically, it may be the flowsheet of choice despite its larger short-term variability in product quality. This illustrates how plants with recycle are generally more difficult to control than units in series.

control structure that does not work

2.7 Ternary System Example

We now move on to study another simple process, but again we gain a considerable amount of insight into some important generic concepts for both process design and control (Tyreus and Luyben, 1993). Here

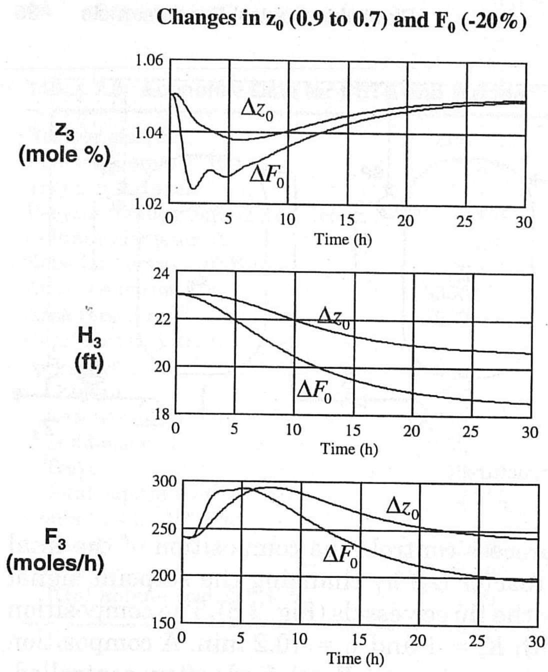

Figure 2.9 Dynamic responses of three-CSTR process.

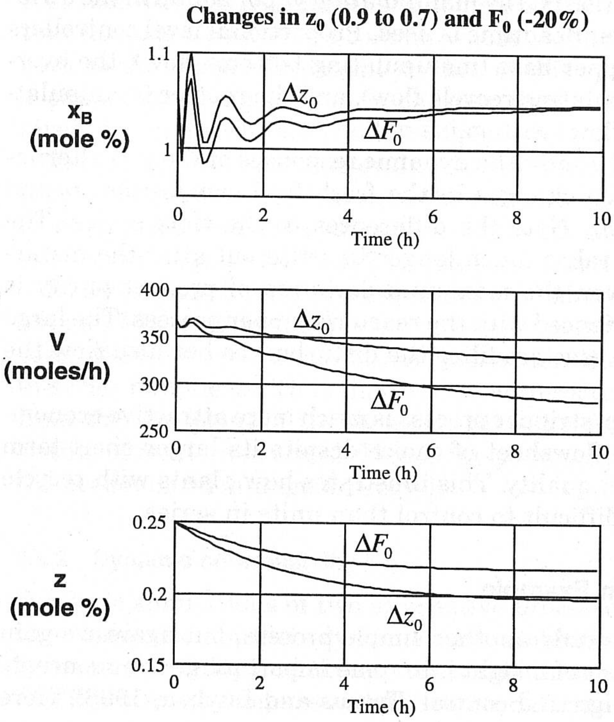

Figure 2.10 Dynamic responses of reactor/stripper process.