CHAPTER 9

Isomerization Process

9.1 Introduction

In the previous chapter we studied a fairly simple process consisting basically of a boiling-liquid reactor and a simple separation section. Although the Eastman process has some plantwide control features, it is essentially just a nonlinear reactor control problem. The gas recycle loop acts like a big stirrer. The management of chemical components through fresh feed makeup streams and product streams is the principal aspect that illustrates plantwide control considerations.

In this and the next two chapters, we study more realistically complex chemical processes. These processes feature multiple unit operations connected together with recycle streams.

We begin here with a very simple isomerization process that is similar to some of the simplified processes studied in Chap. 2. The process consists of a reactor, two distillation columns, and a liquid recycle stream. There are four components to consider. In subsequent chapters we look at processes with many more units, many more components, and multiple recycle streams.

Figure 9.1 shows the flowsheet of the isomerization process to convert normal butane (nC_4) into isobutane (iC_4).

$$nC_4 \rightarrow iC_4 \qquad (9.1)$$

This process is quite important in the petroleum industry because isobutane is usually more valuable as a chemical feedstock than normal butane. The typical amount of iC_4 contained in crude oil and produced in refinery operations such as catalytic cracking is sometimes not enough to satisfy the demand. On the other hand the supply of nC_4 sometimes exceeds the demand, particularly in the summer when less nC_4 can be blended into gasoline because of vapor pressure limitations.

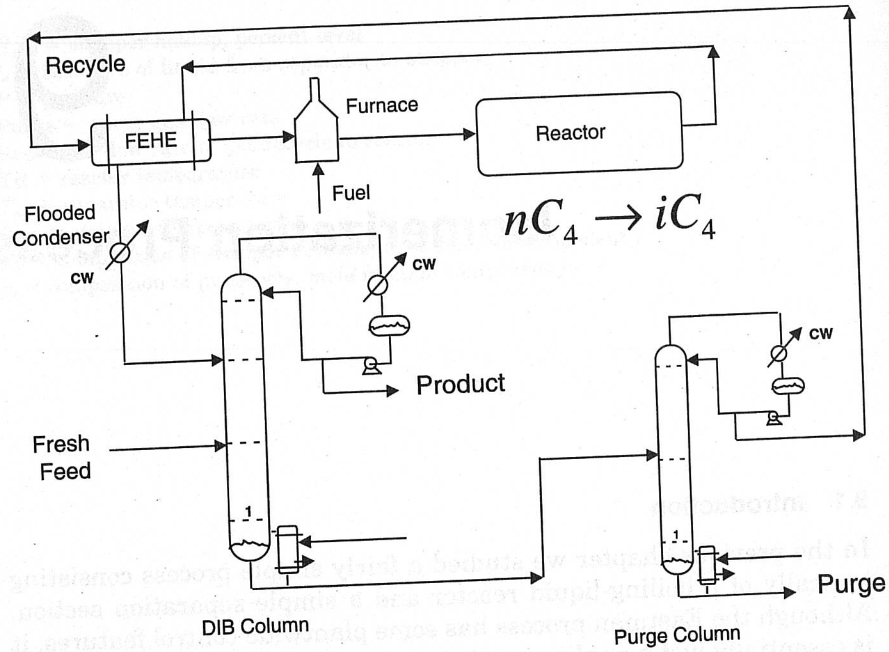

Figure 9.1 Isomerization process flowsheet.

Some of the many uses of isobutane include the production of high-octane gasoline blending components by reacting it with various olefins in alkylation processes and the production of propylene oxide and tertiary butyl alcohol.

The reaction of nC_4 to iC_4 occurs in the vapor phase and is run at elevated temperatures (400°F) and pressures (600 psia). The reaction is exothermic (heat of reaction -3600 Btu/lb · mol), so there is a temperature rise as the process stream flows through the adiabatic tubular reactor. Following heat exchange with the reactor inlet stream and condensation with cooling water, the reactor effluent is introduced into a large distillation column that separates the C_4's. The iso/normal separation is difficult because of the similar relative volatilities, so many trays (50) and a high reflux ratio (7) are required. For the design case considered, this column ends up being 16 feet in diameter. This column is called a *deisobutanizer* (DIB).

The fresh feed stream is a mixture of both nC_4 and iC_4 (with some propane and isopentane impurities). It is also introduced into the column, not directly into the reactor. It is fed at a lower tray in the column than the reactor effluent stream because the concentration of iC_4 in the fresh feed is lower. This enables the removal of some of the iC_4 and all of the C_3 in the fresh feed before sending the nC_4 to the reactor from

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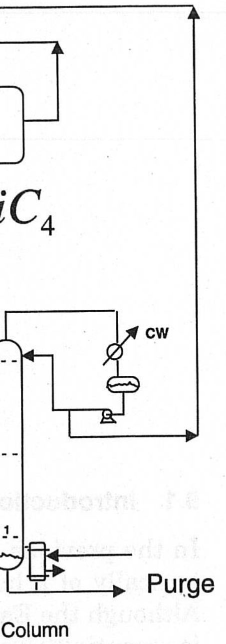

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the recycle stream. The ratio of the recycle flow to the fresh feed flow is about 1:2. The DIB column operates at 100 psia so that cooling water can be used in the condenser (reflux drum temperature is 124°F). The base temperature is 150°F, so low-pressure steam can be used.

The distillate product from the DIB is the isobutane product. It has a specification of 2 mol % nC_4. Since the fresh feed contains some propane, there is also some propane in the distillate product. All of the propane in the feed leaves the process in the distillate stream.

The bottoms from the DIB contains most of the nC_4, along with some iC_4 impurity and all of the heavy isopentane impurity. Since this heavy component will build up in the process unless it is removed, a second distillation column is used to purge out a small stream that contains the isopentane. Some nC_4 is lost in this purge stream. The purge column has 20 trays and is 6 ft in diameter. The distillate product from the second column is the recycle stream to the reactor, which is pumped up to the required pressure and sent through a feed-effluent heat exchanger and a furnace before entering the reactor in the vapor phase.

The numerical case studied is derived from a flowsheet given in Stanford Research Institute Report 91, "Isomerization of Paraffins for Gasoline." Since no kinetic information is given in this report, only reactor inlet and exit conditions, we will assume two different types of kinetics. In Case 1 we consider that the reaction is irreversible. An activation energy of 30,000 Btu/lb · mol is used, and the preexponential factor is adjusted to give the same conversion reported in the SRI report. In Case 2 we assume that the reaction is reversible. The equilibrium constant decreases with increasing temperature because the reaction is exothermic. We also increase the size of the reactor so that the effluent leaves essentially at chemical equilibrium.

These artificial kinetics are used so that a comparison can be made of processes with reversible and irreversible reactions. In particular we want to demonstrate that the effect of increasing reactor temperature is completely different in these two cases. With irreversible reactions, increasing temperature increases production rate. With reversible reactions, increasing temperature can produce a decrease in production rate. Figure 9.2 gives conditions at the Case 1 steady state. Table 9.1 gives stream data for both cases. Table 9.2 lists the process parameter values.

9.2 Plantwide Control Strategy

Step 1. In this process we want to achieve the desired production rate and control the impurity of normal butane in the isobutane product at 2 mol %. Reactor pressure cannot exceed the design operating pressure

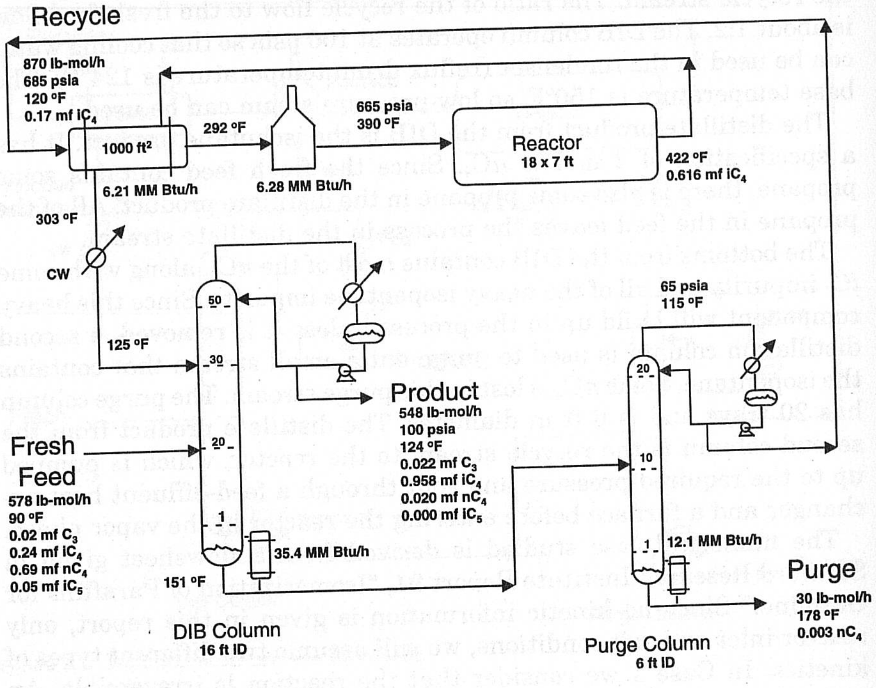

Figure 9.2 Steady-state conditions.

of 700 psia. We assume that we are free to choose the production rate handle. Neither the fresh feed nor product flowrates are fixed by other plant considerations. In the pentane purge column, we do not want to lose too much nC_4.

Step 2. This process has 14 control degrees of freedom. They include: fresh feed valve; DIB column steam, cooling water, reflux, distillate, and bottoms valves; purge column steam, cooling water, reflux, distillate, and bottoms valves; furnace fuel valve; flooded condenser cooling water valve; and DIB column feed valve.

Step 3. The exothermic heat of reaction must be removed, and the reactor feed must be heated to a high enough temperature to initiate the reaction. Since the heat of reaction is not large and complete one-pass conversion is not achieved, the reactor exit temperature is only 32°F higher than the reactor inlet temperature. Since heat transfer coefficients in gas-to-gas systems are typically quite low, this small temperature differential would require a very large heat exchanger if only the reactor effluent is used to heat the reactor feed and no furnace

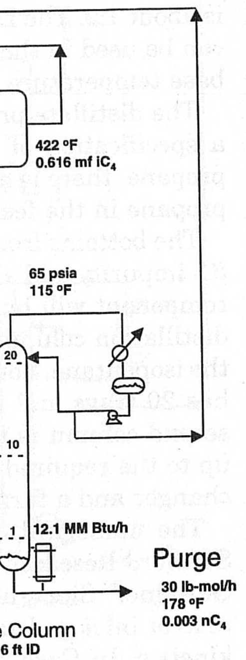

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TABLE 9.1 Stream Data

Case 1 (irreversible reaction)	Fresh feed	Product	Purge	Reactor inlet	Reactor outlet
Flow, lb · mol/h	580	550	30	870	870
Mole fraction C_3	0.02	0.021	0	0	0
Mole fraction iC_4	0.24	0.959	0	0.17	0.62
Mole fraction nC_4	0.69	0.020	0.01	0.81	0.36
Mole fraction iC_5	0.05	0	0.99	0.02	0.02
Temperature, °F	90	124	178	390	422
Pressure, psia	300	100	66	665	650

Cases 1 and 2	Furnace	Flooded condenser	DIB reboiler	Purge reboiler	Reflux flow
Duty, 10^6 Btu/h	6.3	7.3	35.4	12.1	
DIB, lb · mol/h					4000
Purge, lb · mol/h					700

Case 2 (reversible reaction)	Fresh feed	Product	Purge	Reactor inlet	Reactor outlet
Flow, lb · mol/h	544	514	30	870	870
Mole fraction C_3	0.02	0.021	0	0	0
Mole fraction iC_4	0.24	0.959	0	0.17	0.59
Mole fraction nC_4	0.69	0.020	0.01	0.82	0.40
Mole fraction iC_5	0.05	0	0.99	0.01	0.01
Temperature, °F	90	124	178	390	420
Pressure, psia	300	100	66		

is used. Therefore, a furnace is required to bring the reactor inlet temperature up to the desired level.

The use of a feed-effluent heat exchanger (FEHE) reduces the amount of fuel burned in the furnace, as discussed in detail in Chap. 5. So from a steady-state viewpoint, the economic trade-off between utility and capital costs would produce a fairly large heat exchanger and a small furnace. However, the exothermic heat of reaction and the heat of vaporization supplied in the furnace must be dissipated to utilities at the flooded condenser. If the FEHE is too large, reactor heat will be recycled. Also, the larger the heat exchanger, the smaller the heat input in the furnace. This means that we have a smaller handle to deal with disturbances. This could potentially be solved using a bypass around the FEHE on the cold side as discussed in Chap. 5. This should enable us to prevent reactor runaway to high temperature and would guarantee that the furnace is in operation at all times. However, unless the furnace is large enough, there is no guarantee that the system will never quench to low temperature when a large disturbance occurs to drop the reactor inlet temperature.

TABLE 9.2 Parameter Values

		Case 1	Case 2
Reactor	ID, ft	7	7
	Length, ft	18	50
	Holdup, ft^3	693	1925
FEHE	Area, ft^2	1000	1000
	Shell holdup, ft^3	21	21
	Tube holdup, ft^3	21	21
DIB	ID, ft	16	16
	Total trays	50	50
	Feed trays	20/30	20/30
	Reflux ratio	7.3	7.8
	Reflux drum holdup, ft^3	1700	1700
	Base holdup, ft^3	2000	2000
Purge column	ID, ft	6	6
	Total trays	20	20
	Feed tray	11	11
	Reflux ratio	0.8	0.8
	Reflux drum holdup, ft^3	370	370
	Base holdup, ft^3	400	400
Flooded Condenser	Holdup, ft^3	340	340
Kinetics	A_F, 1/h	4×10^8	4×10^8
	E_F, Btu/lb · mol	3×10^4	3×10^4
$K_{EQ} = e^{(A+B/T)}$	A		-10
	B, °R		5000

A second difficulty that can occur with a large FEHE is a hydraulic problem. The recycle stream entering the heat exchanger is a subcooled liquid (115°F) at the pressure in the reactor section (685 psia). As this stream is heated to the required reactor inlet temperature of 390°F, it begins to vaporize. It is superheated vapor when fed into the reactor (390°F at 665 psia). When a small FEHE is used, the exit temperature is 292°F for the recycle stream, which means the stream is still all liquid. All the vaporization occurs in the furnace. If a large heat exchanger were used, vaporization would begin to occur in the heat exchanger. This would make the hydraulic design of this FEHE much more difficult. The dynamic response could also be adversely affected as changes in flowrates and temperature make the stream go in and out of the two-phase region.

The same problem occurs on the hot side of the FEHE. As the hot reactor effluent is cooled, it starts to condense at some temperature. And this dewpoint temperature could occur in the heat exchanger and not in the flooded condenser if a large area is used.

Because of both the heat dissipation and hydraulic concerns, we use a relatively small FEHE: 1000 ft^2 compared to the Stanford Research Report's listed area of 3100 ft^2. So the energy management system consists of controlling reactor inlet temperature by furnace firing and controlling the rate of heat removal in the flooded condenser by cooling water flowrate. The heat of reaction and the heat added in the furnace are therefore removed in the flooded condenser. Because of this design we do not need a bypass around the FEHE.

Step 4. We are not constrained either by reactant supply or product demand to set production rate at a certain point in the process. We need to examine which variables affect reactor productivity.

The kinetic expression for the isomerization reaction is relatively simple. For the irreversible case, reaction rate depends upon the forward rate constant, reactor volume, and normal butane concentration $\mathcal{R} = k_F V_R C_{n\mathrm{C}_4}$. From this expression we see that only three variables could possibly be dominant: temperature, pressure, and mole fraction of $n\mathrm{C}_4$ in the reactor feed.

Pressure affects productivity through its influence on the reactant concentration. Since the normal operating reactor pressure is close to the design limit, we are constrained in how much we can move pressure to achieve the desired production rate change. The $n\mathrm{C}_4$ mole fraction in the reactor feed is about 0.81. Therefore large absolute changes in the reactant feed mole fraction would have to be made to achieve a significant relative change in throughput.

Finally, we are then left with temperature. We see from Eq. (4.7) how the relative change in reaction rate depends upon the temperature through the activation energy. In this case the reaction rate increases by 20 percent for a 10°F change in temperature. Clearly temperature is a dominant variable for reactor productivity.

For the reversible case, reaction rate depends upon the forward and reverse rate constants, reactor volume, and $n\mathrm{C}_4$ and $i\mathrm{C}_4$ concentrations:

$$\mathcal{R} = k_F V_R C_{n\mathrm{C}_4} - k_R V_R C_{i\mathrm{C}_4}$$

The activation energy of the reverse reaction is always greater than the activation energy of the forward reaction since the reaction is exothermic. Therefore the reverse reaction will increase more quickly with an increase in temperature than will the forward reaction. Temperature may still dominate for reactor productivity, but in the opposite direction compared with the irreversible case, since conversion increases with lower temperature. However, when the temperature becomes too low, both reaction rates slow down such that we cannot achieve the desired production rate with this variable alone. Instead, the concentrations of $n\mathrm{C}_4$ and $i\mathrm{C}_4$ dominate the rate through the relationship imposed by the equilibrium constant $K_{\mathrm{eq}} = C_{i\mathrm{C}_4}/C_{n\mathrm{C}_4}$.

Therefore we choose the reactor inlet temperature setpoint as the production rate handle for the irreversible case. However, for the reversible case we need to look for variables that affect the ratio of $n\text{C}_4$ to $i\text{C}_4$ in the recycle stream. For this case we will not have unit control for the reactor since these concentrations depend upon operation in other parts of the process.

Note that setting the production rate with variables at the reactor or within the process specifies the amount of fresh reactant feed flow required at steady state. The choices for the control system made in Steps 6 and 7 must recognize this relationship between production rate and fresh reactant feed flowrate.

Step 5. The final isobutane product is the distillate from the DIB column, and we want to keep the composition of the $n\text{C}_4$ impurity at 2 mol %. Nothing can be done about the propane impurity. Whatever propane is in the fresh feed must leave in the product stream. Because the separation involves two isomers, the temperature profile is flat in the DIB column. Use of an overhead composition analyzer is necessary.

The choices of manipulated variables that can be used to control $n\text{C}_4$ composition in the DIB distillate include reflux flowrate, distillate flowrate, and reboiler heat input. Because the reflux ratio is high, control of reflux drum level using distillate flow may be ineffective, particularly if the distillate were going directly to a downstream process. If we decide to use reflux flow to control reflux drum level, we must control distillate composition by manipulating the distillate flowrate. The reason is that distillate flow must match production rate, which is independently set in the reactor. However, in this case we assume that the distillate is going to a storage tank or cavern, so large changes in distillate flowrate are not important. Distillate can then be used for reflux drum level control, allowing us to consider other variables for composition control.

Most distillation columns respond more quickly to vapor rate changes than to changes in liquid rates. Therefore, we select reboiler heat input to control $n\text{C}_4$ impurity in the distillate. This may seem like a poor choice because we are controlling something at the top of the column by changing a variable near the base. However, vapor changes affect all trays in the column quite quickly, so tight control of distillate composition should be possible by manipulating vapor boilup. A viable alternative is to control distillate composition with distillate flowrate and control reflux drum level with reflux flowrate.

For the reversible case, we are interested in the composition of the bottoms stream from the DIB column. We may consider dual composition control (controlling both the $n\text{C}_4$ impurity in the top and the $i\text{C}_4$ impurity in the bottom). Logic would dictate that the distillate composi-

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tion should be controlled by manipulating the distillate flowrate and bottoms composition should be controlled by manipulating heat input.

To avoid the high-pressure safety constraint, we must control reactor pressure. We can use the distillate valve from the purge column, the flooded condenser cooling water valve, or the DIB column feed valve. The most logical variable to use for control of the flooded condenser (reactor) pressure is the DIB column feed valve (as shown in Fig. 5.5). Based upon the discussion in Step 3, we would then use the flooded condenser cooling water valve to keep the liquid level in a good control range.

Step 6. We have only two choices, DIB column base valve or purge column distillate valve, for fixing a flow in the recycle loop. Either of these would work. The rationale for picking one is based upon avoiding disturbances to the unit downstream of the fixed flow location. Since the purge column is not critical from the viewpoint of product quality, we elect to fix the flow upstream of reactor (purge column distillate flow) so that we minimize disturbances in reactor temperature and pressure.

We must control the two column pressures. As discussed in Chap. 6, this is best done by manipulating the condenser cooling water flowrates.

There are four liquid levels to be controlled. DIB column reflux drum level is controlled by manipulating distillate product flowrate. We must also control the levels in the DIB column base and in the purge column reflux drum and base.

Having made the choice to fix the purge column distillate flow, we are faced with the problem of how to control purge column reflux drum level. We have two primary choices: reflux flow or heat input. We choose the latter because the flowrate of the purge column reflux is small relative to the vapor coming overhead from the top of the column. Remember the Richardson rule, which says we select the largest stream.

The flowrate of the purge stream from the base of the purge column is quite small, so it would not do a good job in controlling base level. This is especially true when the large steam flow has been selected to control the reflux drum level. Base level in the purge column can, however, be controlled by manipulating the bottoms flowrate from the DIB column.

We are then left with controlling base level in the DIB column. The only remaining valve is the fresh nC_4 feed flowrate into the column. The feed is liquid and there are only 20 trays between the lower feed point and the column base, so base level control using feed should be possible. This base level is also an indication of the nC_4 inventory within the process.

The material balance control structure works opposite to the direction of flow. Purge column distillate is fixed; purge column reflux drum level is controlled by vapor boilup; purge column base level is controlled by the feed to the purge column; and DIB column base level is controlled by the fresh feed to the DIB column.

Had we started to assign the DIB column base level control first, we would have ended up with the same inventory control structure. The reason is as follows. Assume we had chosen the DIB column base valve to control base level. After resolving the purge column inventory loops, we would have found that we needed to control the purge column base or reflux drum level with the fresh feed flow to the DIB column. The dynamic lags associated with these loops would have forced us back to the control strategy as described above.

An obvious question at this point is "Why don't we just flow control the fresh feed into the process?" If we did this, we could not fix the flowrate in the recycle loop. For example, suppose we select the following control structure: fix fresh feed flowrate, control DIB column base level with DIB bottoms, control purge column base level with heat input, and control purge column reflux drum level with distillate. This structure is intuitively attractive and permits us to fix the production rate directly by setting the fresh feed flowrate. However, only level controllers set the flows around the recycle loop, so we would expect problems with snowballing. Flow disturbances can propagate around the liquid recycle loop. Simulation results given later in this chapter demonstrate that this is indeed what occurs with this structure. It does not give stable regulatory control of the process.

Step 7. Four components need to be accounted for. The light inert propane leaves in the product stream. The heavy inert component isopentane (iC_5) leaves in the purge stream. Any iC_4 coming into the process in the fresh feed and the iC_4 produced by the reaction can leave in the product stream.

The only component that is trapped inside the system and must be consumed by the reaction is nC_4. The composition controller on the DIB distillate stream permits only a small amount (2 mol %) of nC_4 to leave in the product stream. The purge stream from the bottom of the purge column permits only a small amount of nC_4 to escape. This purge stream can be simply flow-controlled if we don't mind losing a small amount of nC_4 with the iC_5 purge. If the amount of iC_5 in the fresh feed is small, this may be the simplest strategy and may have little economic penalty. Alternatively we could control the amount of nC_4 in the purge column bottoms by manipulating bottoms flowrate. Since there is a fairly large temperature change in the purge column, controlling the temperature on a suitable tray (tray 2) may be more practical since it eliminates the need for an on-line analyzer. In the simulations given later in this chapter, we adopt the simple strategy of flow-controlling the purge stream.

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The amount of reactant nC_4 fed into the system must somehow be exactly balanced by the amount of nC_4 converted to product iC_4. The process acts almost like a pure integrator in terms of the moles of nC_4. The way this balancing of nC_4 is accomplished in the control structure shown in Figure 9.3 is by using the level in the base of the DIB column to indicate if the nC_4 is building up in the system or is being depleted. The material in the DIB base is mostly nC_4. There is a little iC_4 (16 percent) and a little iC_5 (5 percent), and the remainder is nC_4. So DIB base level changes reflect changes in nC_4 inventory in the process. If this level is increasing, fresh feed flowrate should be reduced because we are not consuming all the reactant being fed into the process. If the level is decreasing, fresh feed flowrate should be increased because we are consuming more reactant than we are feeding.

Table 9.3 summarizes the component balance control strategy.

Step 8. The previous steps have left us at this point with two unassigned control valves, which are the reflux flows to each column. As discussed in Chap. 6, these are independent variables and can be fixed by flow controllers. We do not need dual composition control for the irreversible case because only one end of both columns is a product stream leaving the process. These two reflux flowrates are available in Step 9 to use as optimizing variables or to improve dynamic response. However, we may need dual composition control in the DIB column for the reversible case as mentioned in Steps 4 and 5.

Step 9. When we use reactor inlet temperature for production rate control (irreversible case), the only remaining degrees of freedom for optimization are the reflux flows for the two columns and the setpoint of the distillate flowrate from the purge column (recycle flow).

In the reversible case, when the base composition of the DIB column or the recycle flowrate is used for production rate control, the remaining degrees of freedom are purge column reflux flow and the reactor inlet temperature.

9.3 Dynamic Simulations

The simulation of this process was constructed using the commercial simulator from Hyprotech Ltd. A copy of the case "isom.hsc" can be obtained from the Web page of William L. Luyben at Lehigh University at the following site: *wll0@lehigh.edu*.

In the HYSYS simulation, the flooded condenser is simulated as a cooler with a temperature control loop manipulating cooling water rate. The reactor inlet pressure is set by the exit of the liquid recycle pump on the purge column distillate stream.

All level controllers are proportional only with a gain of 2. Tempera-

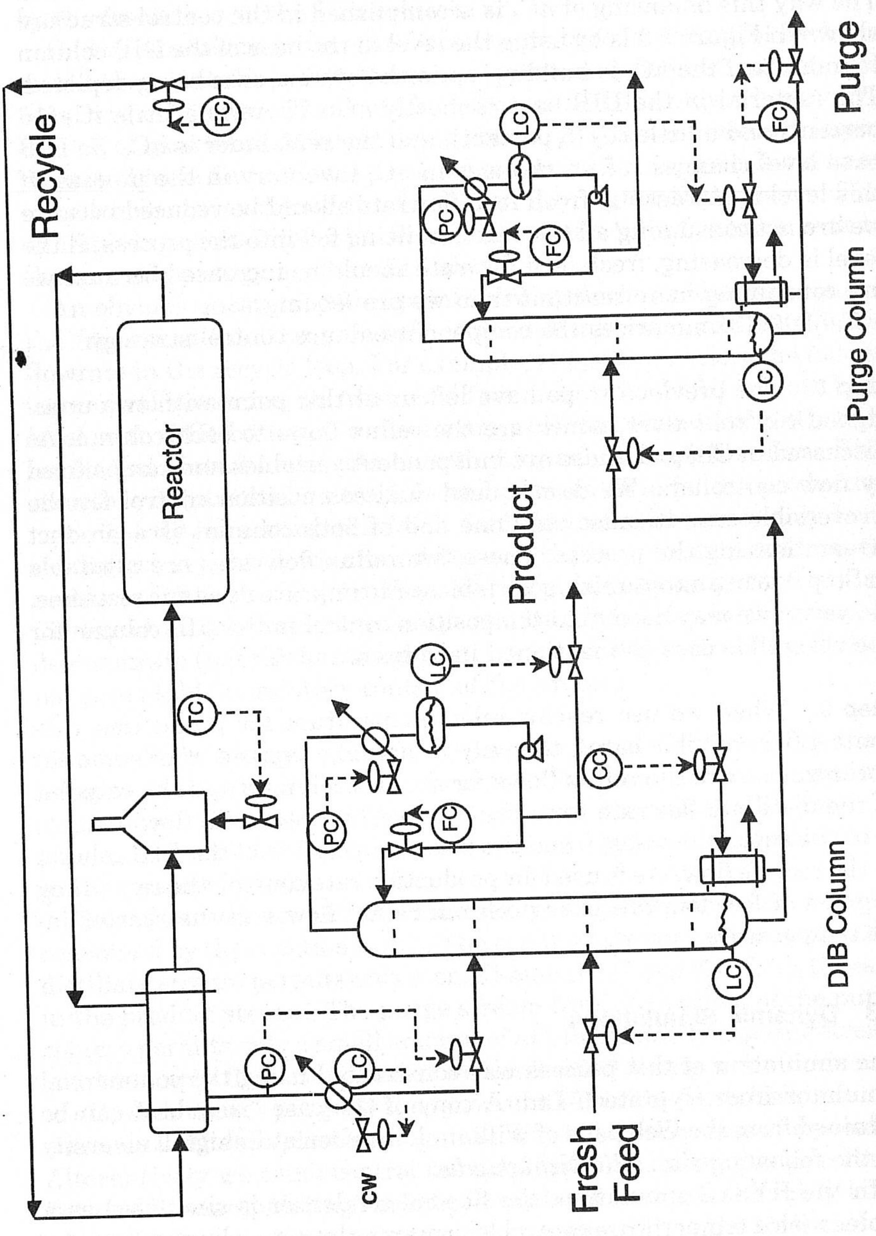


Figure 9.3 Control structure for isomerization process.

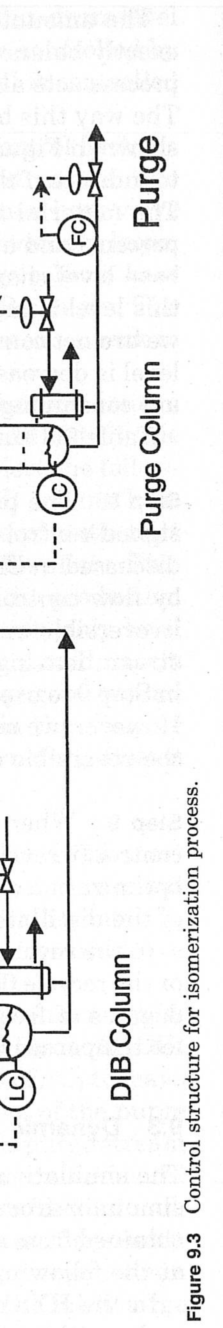


Figure 9.3 Control structure for isomerization process.

TABLE 9.3 Component Material Balance for Irreversible Case

Component	Input	+Generation	−Output	−Consumption	=Accumulation Inventory controlled by
C_3	Fresh feed	0	Product stream	0	Self-regulating by product quality controller
iC_4	Fresh feed	$k_F V_R C_{nC4}$	Product stream	0	Controlled by product quality controller
nC_4	Fresh feed	0	0	$k_F V_R C_{nC4}$	Indicated by DIB column base level
iC_5	Fresh feed	0	Purge stream	0	Self-regulating by composition change in purge

ture and composition controllers are tuned using the TL settings after the ultimate gain and frequency are obtained via relay-feedback tests. Two temperature measurement lags of 0.1 minute are included in the two temperature loops (reactor inlet temperature and DIB feed temperature). A 3-minute deadtime is assumed in the product composition measurement (distillate from the DIB). Table 9.4 gives valve and transmitter spans and controller tuning constants.

Rigorous dynamic simulations of the irreversible reaction case and the reversible reaction case permit us to evaluate how effective the

TABLE 9.4 Control Parameters

Reactor inlet temperature controller	Valve span, 10^6 Btu/h	15
	Transmitter span, °F	200
	K_c	2
	Reset, minutes	10
Cooler temperature controller	Valve span, 10^6 Btu/h	20
	Transmitter span, °F	100
	K_c	1
	Reset, minutes	10
Temperature measurement lags (two)	Time constant, minutes	0.1
Product composition controller	Valve span, 10^6 Btu/h	50
	Transmitter span, mole fraction nC_4	0.1
	K_c	1
	Reset, minutes	60
Composition deadtime	minutes	3
Level controllers	K_c	2

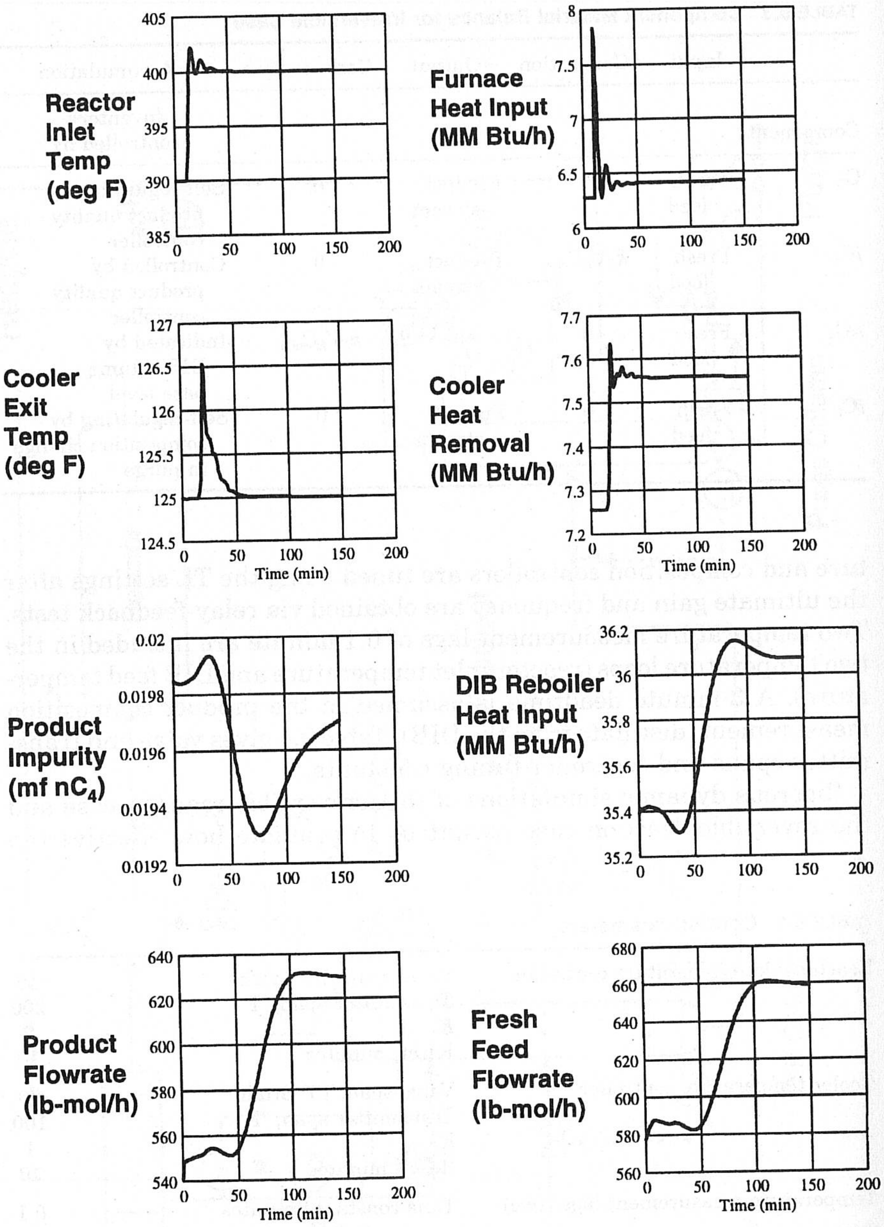
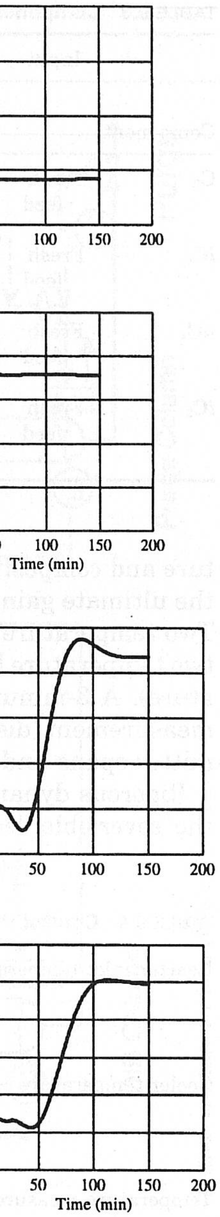


Figure 9.4 Irreversible reaction case dynamic response to 10°F increase in reactor inlet temperature.



ncrease in reactor in-

control structure is. These simulations also alert us to any potentially difficult dynamics that would indicate tuning problems or a need to provide more surge capacity for some of the inventory loops. As we expected, the simulations show that the control strategy works and provides good base-level regulatory control.

9.3.1 Irreversible reaction

Figures 9.4 and 9.5 show results for the irreversible reaction case when reactor inlet temperature is changed and when recycle flowrate is changed. Figure 9.4 shows that a 10°F step increase, occurring at time equals 10 minutes, produces an increase in product flowrate (from 550 to 630 lb · mol/h). As more iC_4 is produced in the reactor with the increase in reaction rate at the higher temperature, the purity of the DIB distillate improves (less nC_4 in the overhead product), which causes the reboiler heat input to increase. This lowers the base level, and pulls in more fresh feed. So changing reactor inlet temperature is an effective way to set production rate when the reaction is irreversible.

Figure 9.5 shows the effect of increasing the recycle flowrate from 870 to 1000 lb · mol/h. If no other change is made, the effect is a slight *decrease* in production rate! This is certainly not what we would intuitively expect. This unusual behavior can be explained by consider-

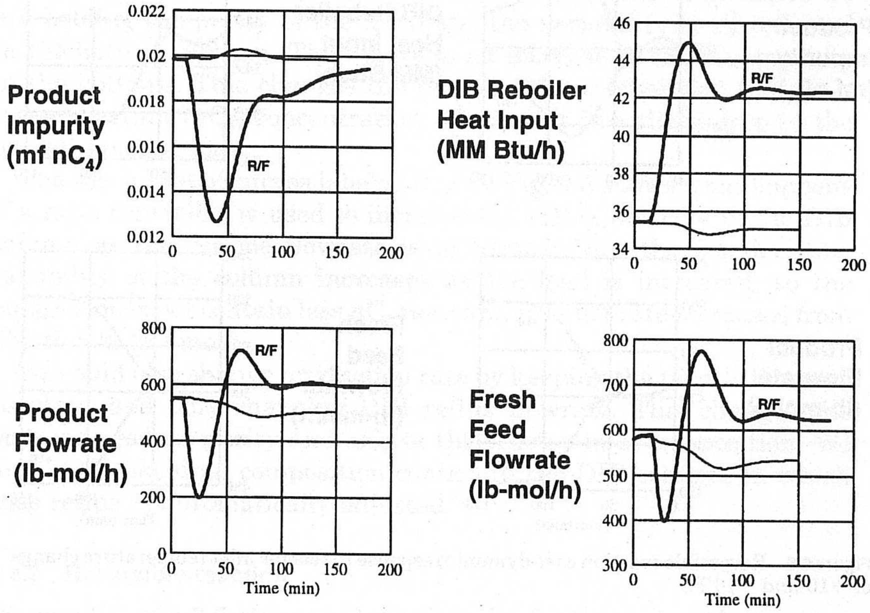


Figure 9.5 Irreversible reaction case dynamic response to increase in recycle flow from 870 to 1000 lb · mol/h (R/F curves indicate constant reflux-to-feed ratio in DIB column).

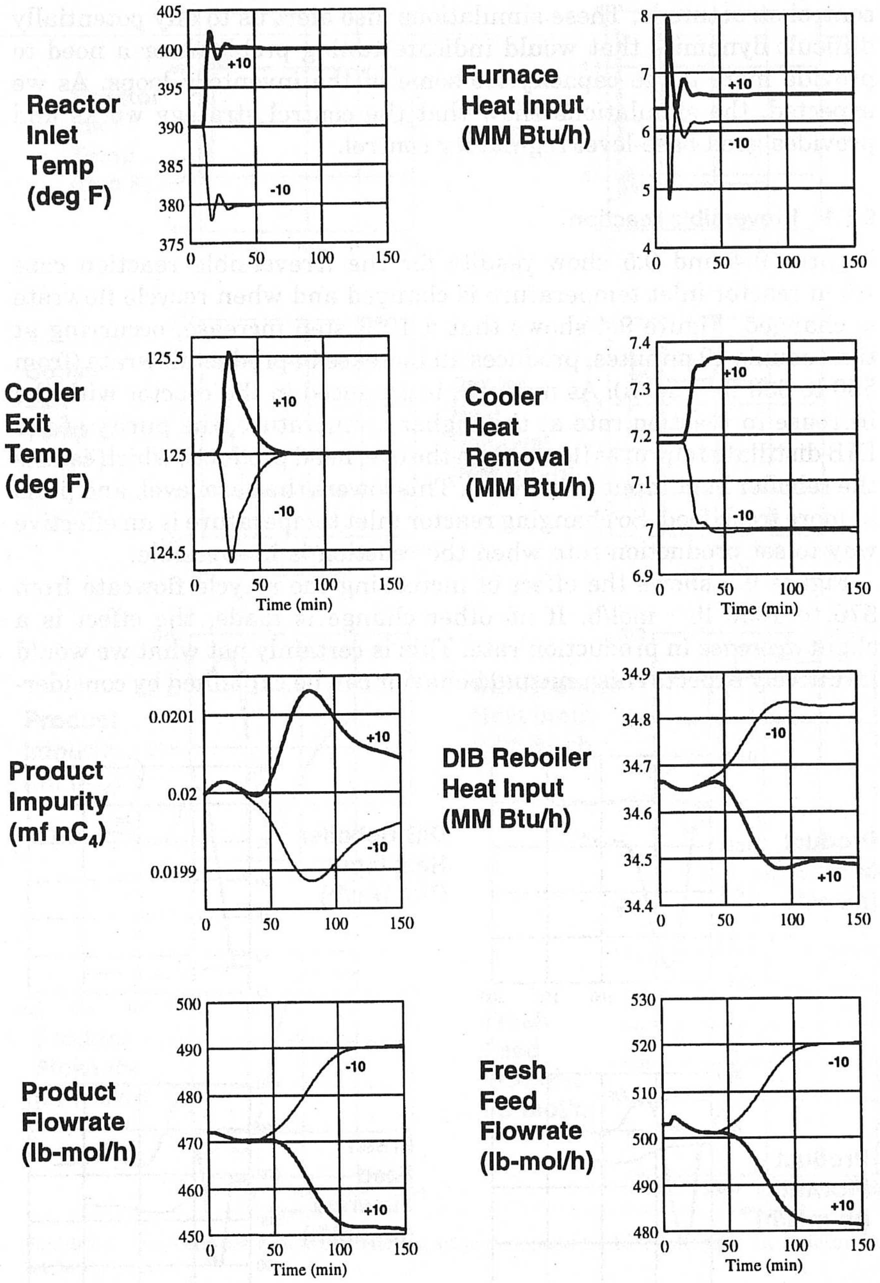
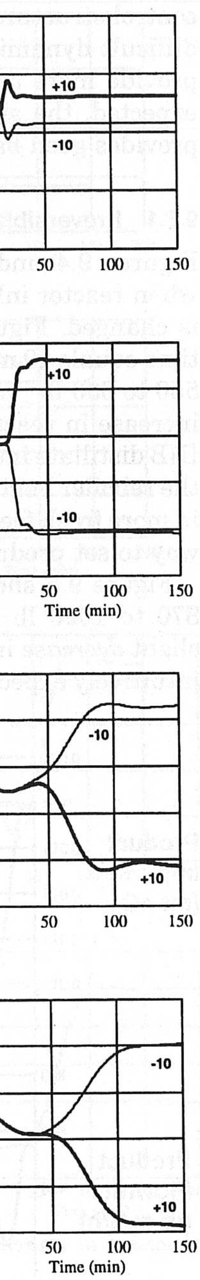


Figure 9.6 Reversible reaction case dynamic response to reactor inlet temperature change of +10 and −10°F.



temperature change

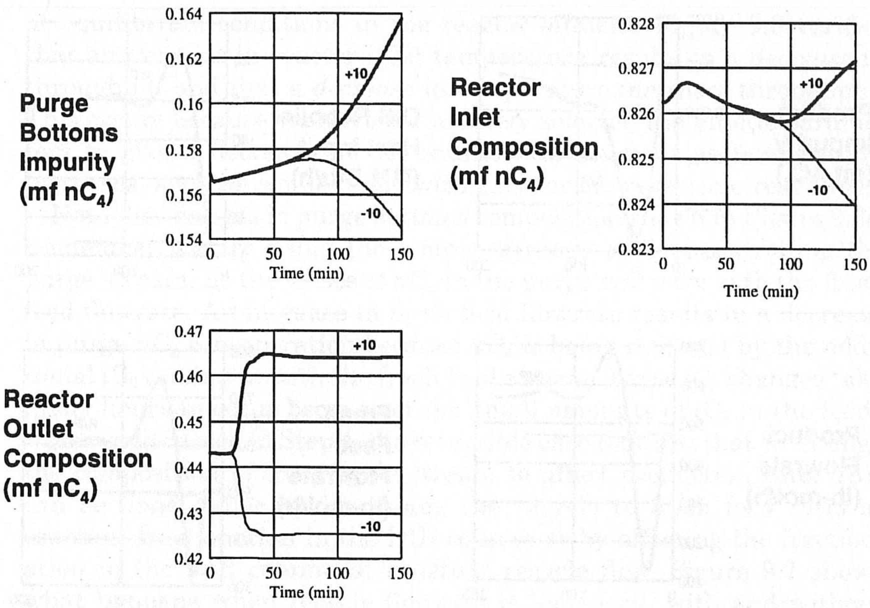


Figure 9.6 *(Continued)*

ing what happens in the DIB column. More recycle means a higher feed rate to this column, which increases the column load. Since we are holding the purity of the distillate, the variability is all reflected in the bottoms stream. Thus there is an increase in the iC_4 impurity in the bottoms. This changes the reactor inlet composition to have a lower reactant (nC_4) concentration. The result is a slight drop in the overall reaction rate.

The second set of curves labeled R/F in Fig. 9.5 shows what happens if a ratio controller is used to increase the reflux flowrate in the DIB column as the recycle flowrate is increased. Now the fractionating capability of the column increases as the load is increased, so the bottoms does not contain less nC_4 reactant. Product rate increases from 550 to 592 lb · mol/h.

We could also change production rate by keeping the recycle flowrate constant and only changing DIB reflux flowrate. This changes the bottoms product purity and affects the reactor inlet composition. We also could use dual composition control in the DIB column, in which case reflux is automatically adjusted.

9.3.2 Reversible reaction

Figures 9.6 and 9.7 give simulation results for the reversible reaction case where a large reactor is used so that the reaction is essentially

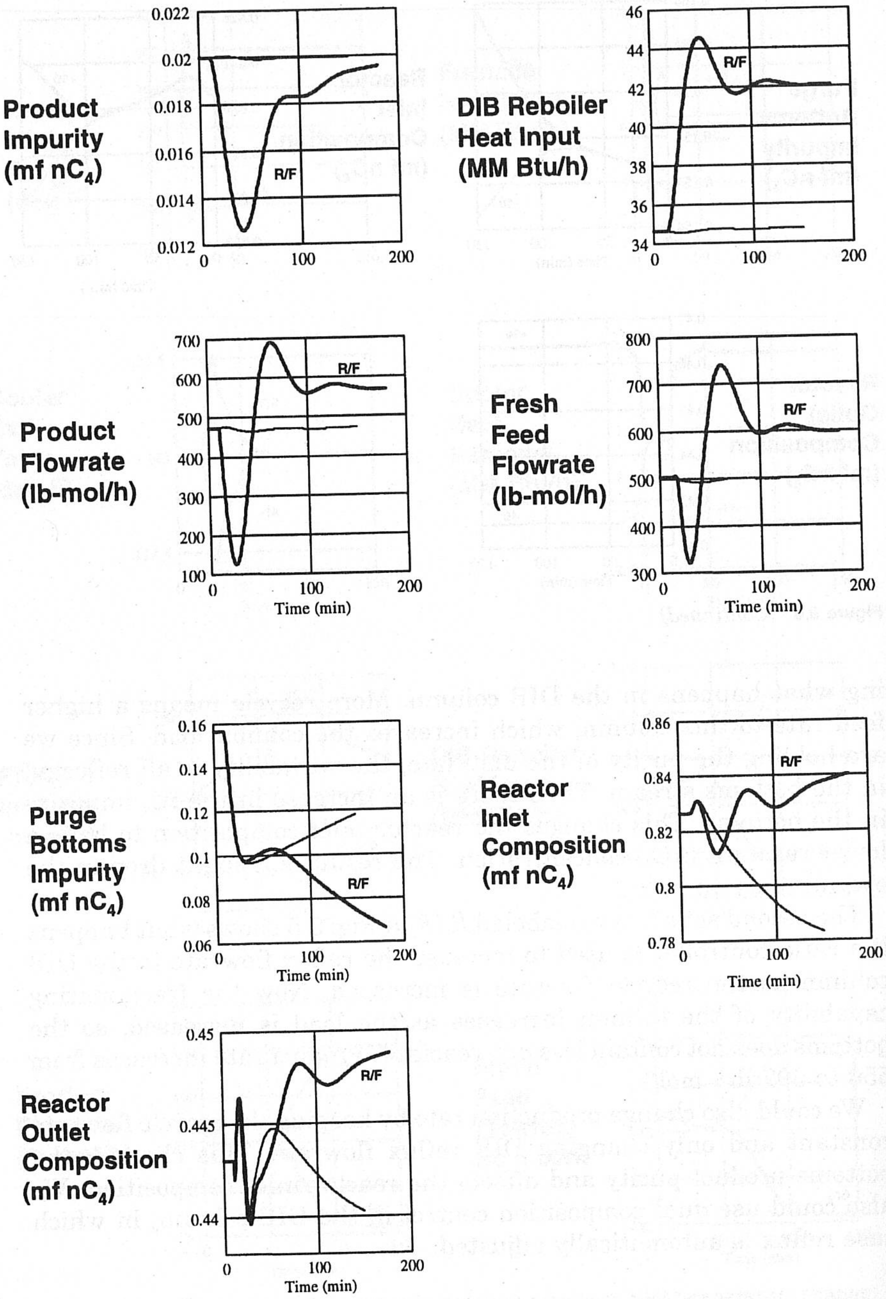
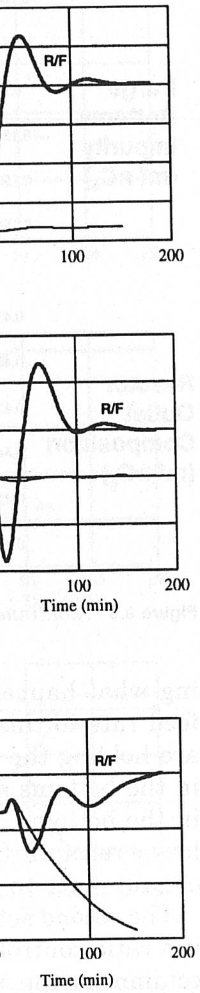


Figure 9.7 Reversible reaction case dynamic response to recycle flow increase (R/F curves indicate constant reflux-to-feed ratio in DIB column).



ncrease (R/F curves

at equilibrium conditions in the reactor effluent. Figure 9.6 verifies that an *increase* in reactor inlet temperature results in a *decrease* in throughput and that a *decrease* in temperature *increases* throughput. This occurs because we have deliberately selected the kinetic parameters to give a decrease in the equilibrium constant as temperature increases, such as would occur with exothermic reversible reactions.

Note the changes in purge bottoms composition shown in Figure 9.6*c*. Remember we are using the simple strategy of flow controlling the purge stream. So the losses of nC_4 in the purge will vary with the fresh feed flowrate. An increase in fresh feed flowrate results in a decrease in purge nC_4 concentration because nC_4 is being replaced by the additional iC_5 coming in with the fresh feed stream. These iC_5 changes take many hours to occur because of the small amounts of iC_5 in the feed.

As we discussed in Step 4, the reversible case requires that we change the composition of the recycle stream to affect production rate. This can be done either by increasing the recycle to fresh feed ratio at constant fractionation in the DIB column or by affecting the fractionation in the DIB column at constant recycle flow. Figure 9.7 shows what happens when recycle flowrate is increased, with and without the reflux-to-feed ratio controller. When only the recycle flowrate is changed, production rate is essentially constant because we are effectively lowering the fractionation in the DIB column. More material is flowing through the reactor, and we would expect to get more iC_4 produced. But the change in the loading of the DIB column shifts the reactor inlet composition (less reactant nC_4). However, when we hold constant the reflux-to-feed ratio, an increase in recycle flow increases production rate.

9.3.3 Fixed fresh feed control structure

Figure 9.8 presents a control structure that most engineers would probably come up with for this process. Each of the units in isolation has standard "textbook" control strategies. Production rate is set by flow-controlling fresh feed to the DIB column. Liquid flows around the recycle loop are set by controlling levels. DIB base level is controlled by manipulating DIB bottoms flow. Reboiler heat input is used to control purge column base level. Purge column reflux drum level is controlled by manipulating distillate flowrate (recycle).

Figure 9.9 shows what happens for the irreversible reaction case. No disturbance is made. The system goes unstable and shuts down when control valve saturation occurs after about 2 hours. The reason for this should not come as a surprise at this point in the book. This "obvious" control strategy has no way to regulate the inventory of nC_4 component within the system.

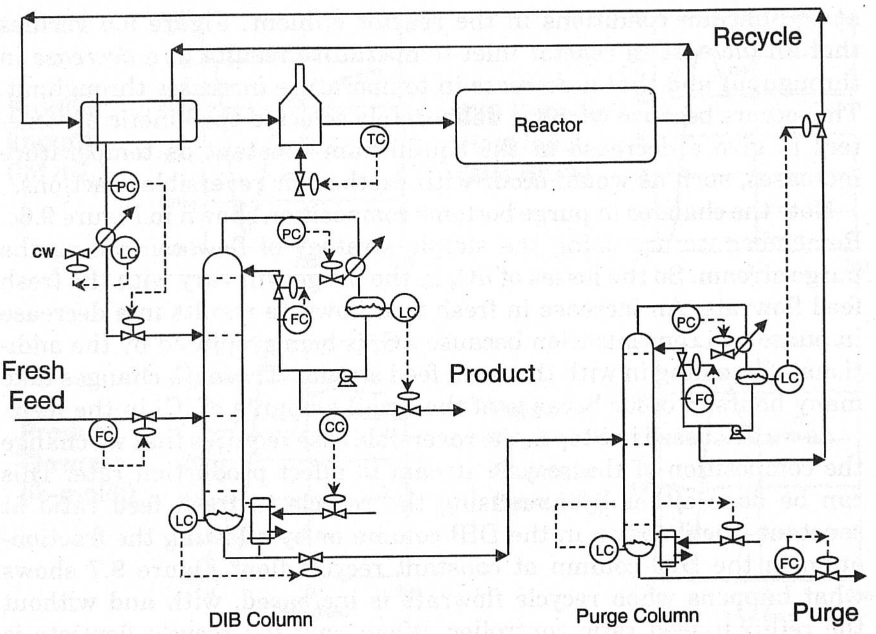


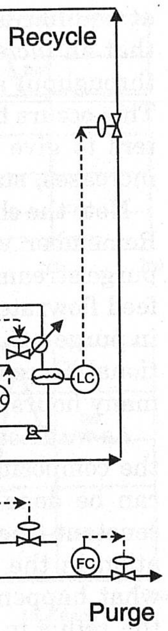
Figure 9.8 Fixed feed control structure.

9.4 Conclusion

The process considered in this chapter is very simple. The reaction involves only one reactant and one product. Two inert components, one light and one heavy, are also present. These inerts must be purged from the system. The major plantwide control consideration is how to adjust the fresh feed of the reactant to balance exactly its rate of consumption by reaction. This is achieved by using the liquid level that is a good indication of the amount of reactant in the system (the base level in the DIB column).

Despite its simplicity, the isomerization process displays some interesting behavior, some expected and some unexpected. The effect of recycle flowrate is probably the most nonintuitive phenomenon: recycle flowrate has little effect on throughput. This results because recycle flowrate affects both the reactor and the separation section, and the net effect is little change in production rate.

In the next two chapters, more complex flowsheets are considered. But many of the fundamental ideas developed in this chapter and in Chap. 2 are directly applicable to these complex, multiunit, multirecycle, multicomponent processes.



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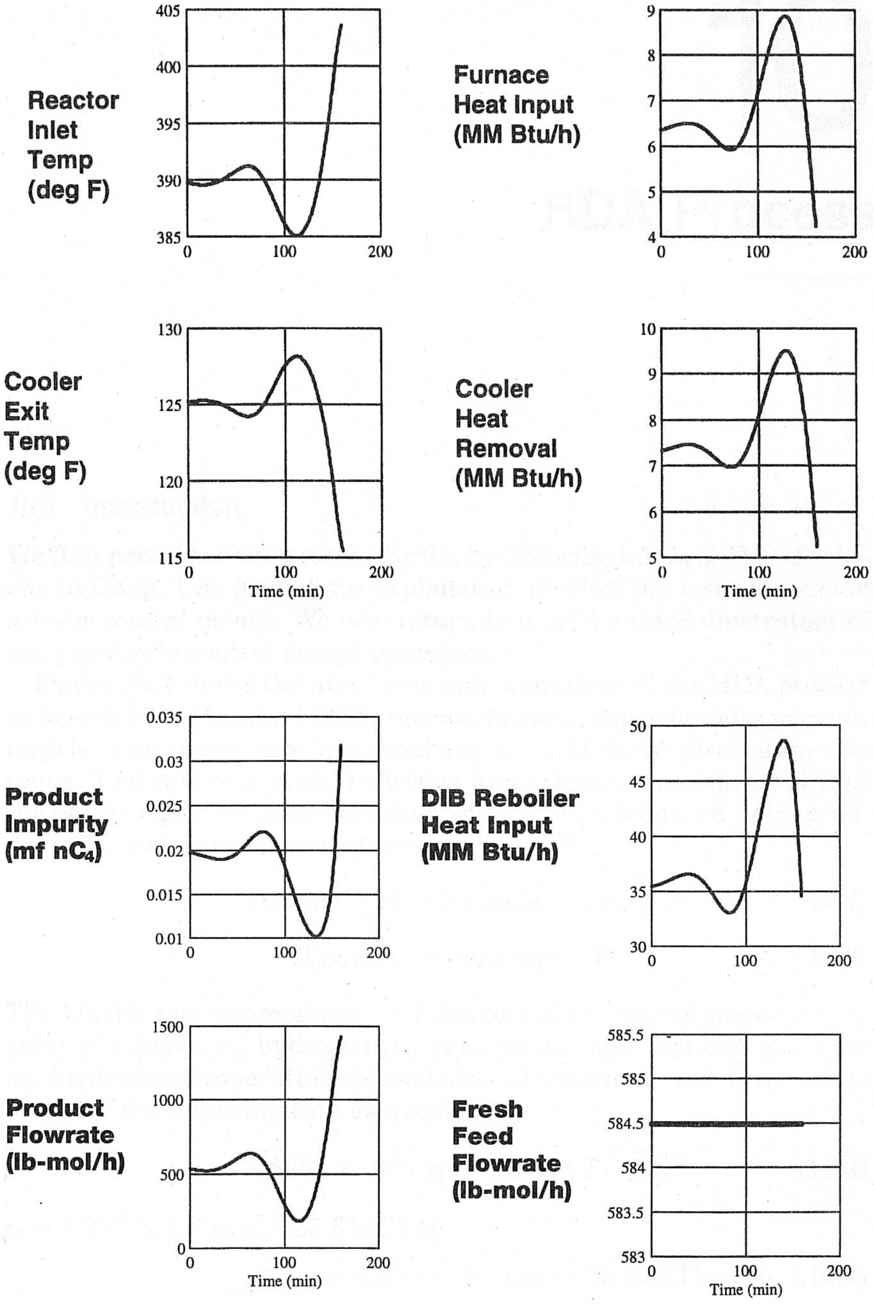

Figure 9.9 Dynamic response of fixed feed control structure for irreversible reaction case.