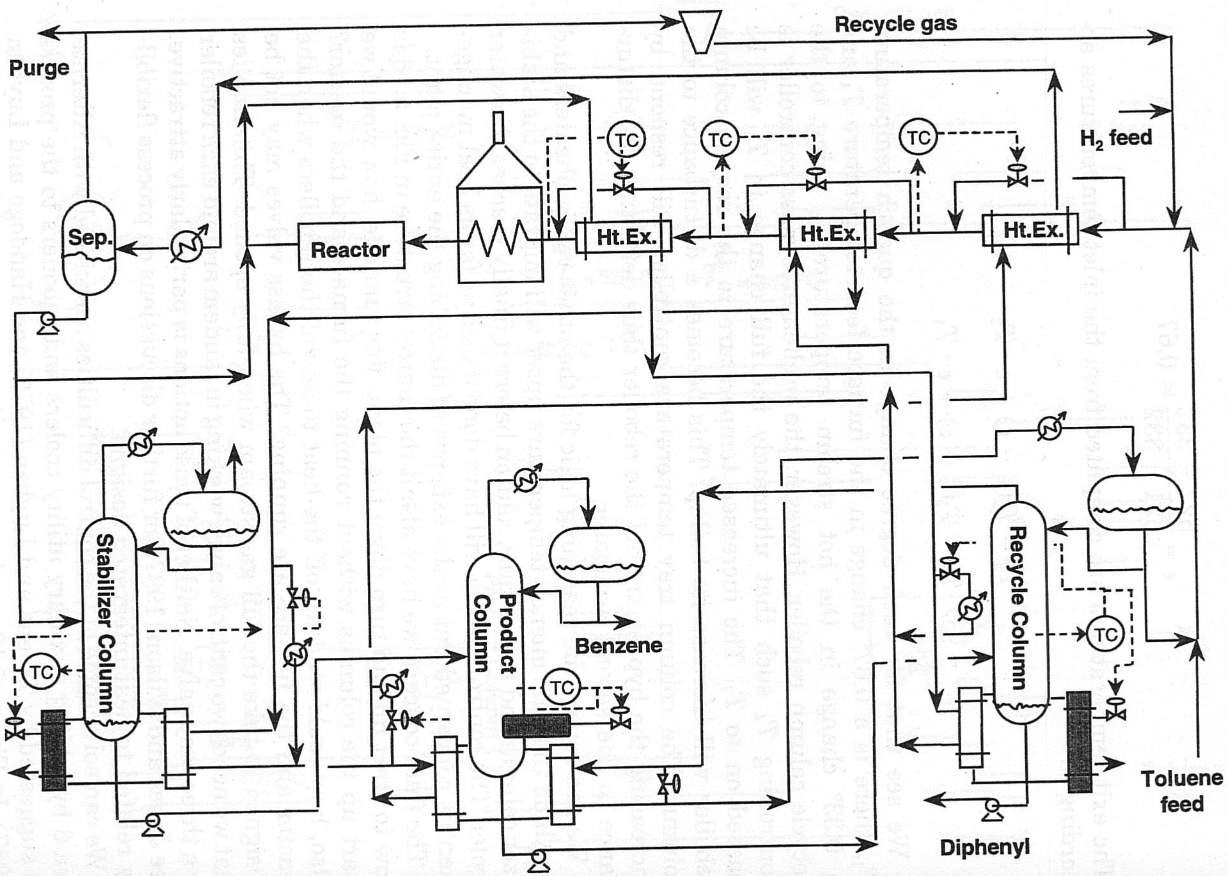


Figure 5.18 HDA process Alternative 6 with complete heat management control system using auxiliary coolers and reboilers.

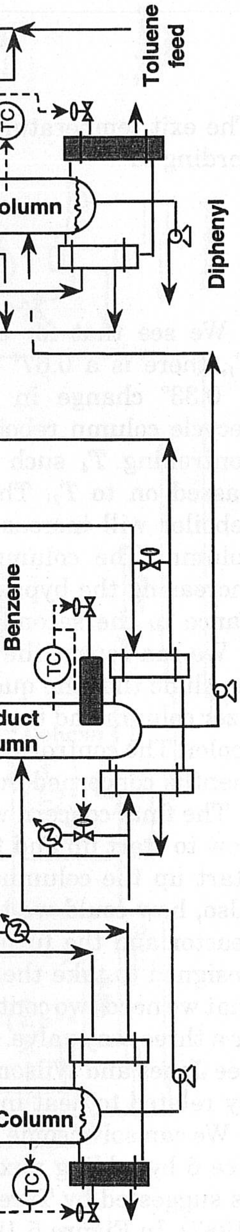


Figure 5.18 HDA process Alternative 6 with complete heat management control system using auxiliary coolers and reboilers.

quickly to utilities without propagating through the entire plant. This is the essence of the rate of exergy destruction principle. Disturbances are rejected to the auxiliary coolers when the column temperature controllers divert excess heat around the main reboilers. The auxiliary reboilers are used to provide a quick source of energy for the columns so that heat deficiencies in the process are not propagated to the next downstream unit operation.

The control system in Fig. 5.18 has a much better chance of providing flexibility and operability than the one shown in Fig. 5.16. However, we have added quite a bit of extra equipment and control valves so the economics of the modified Alternative 6 have to be revisited. In addition, we still have concerns about the design of the hot-gas-heated reboilers and bypass valves for hot hydrogen service. It may be that this level of heat integration is too complicated and ambitious compared to the savings achievable. Simpler designs could be just as profitable when operability is put into the picture. We should recall the 80/20 rule that suggests that we could get 80 percent of the savings with 20 percent of the effort. The base case shown in Chap. 1 and Alternative 1 mentioned earlier represent simpler designs with a healthy level of heat recovery. We therefore take a closer look at the characteristics and control of such alternatives.

5.7 Reactor Feed-Effluent Exchange Systems

5.7.1 Introduction

In Chap. 4 we mentioned that the simplest reactor type from a control viewpoint is the adiabatic plug-flow reactor. It does not suffer from output multiplicity, open-loop instability, or hot-spot sensitivity. Furthermore, it is dominated by the inlet temperature that is easy to control for an isolated unit. The only major issue with this reactor type is the risk of achieving high exit temperatures due to a large adiabatic temperature rise. As we recall from Chap. 4, the adiabatic temperature rise is proportional to the inlet concentration of the reactants and inversely proportional to the heat capacity of the feed stream. We can therefore limit the temperature rise by diluting the reactants with a heat carrier.

While introducing a heat carrier solves the reactor problem, it unfortunately creates some other concerns. First, we increase the size of the separation section since we have to separate the products from a large amount of heat carrier. Second, we make the plant thermally inefficient by significantly increasing the plant's energy load due to repeated heating and cooling of the heat carrier. To solve the efficiency problem we introduce heat integration. As we saw in the HDA example, a healthy improvement in efficiency is achieved by simply preheating the reactor feeds with the hot reactor effluent. These schemes are called *feed-effluent heat exchange* systems, or FEHE systems for short. An FEHE system sometimes has the ability to eliminate all heating and cooling requirements around the reactor and make it autothermal.

It now looks as if we have achieved the best of all worlds: a thermally efficient process with an easy-to-control reactor! Can this be true? Not quite. What we forget are the undesirable effects on the reactor that thermal feedback introduces. In Chap. 4 we explained in detail how process feedback is responsible for the same issues we tried to avoid in the first place by selecting an adiabatic plug-flow reactor. It is necessary that we take a close look at the steady-state and dynamic characteristics of FEHE systems.

5.7.2 Open-loop characteristics

Just as we approached reactor control in Chap. 4, we will start by exploring the open-loop effects of thermal feedback. Consider Fig. 5.19, which shows an adiabatic plug-flow reactor with an FEHE system. We have also included two manipulated variables that will later turn out to be useful to control the reactor. One of these manipulated variables is the heat load to the furnace and the other is the bypass around the preheater. It is clear that the reactor feed temperature is affected by the bypass valve position and the furnace heat load but also by the reactor exit temperature through the heat exchanger. This creates the possibility for multiple steady states. We can visualize the different

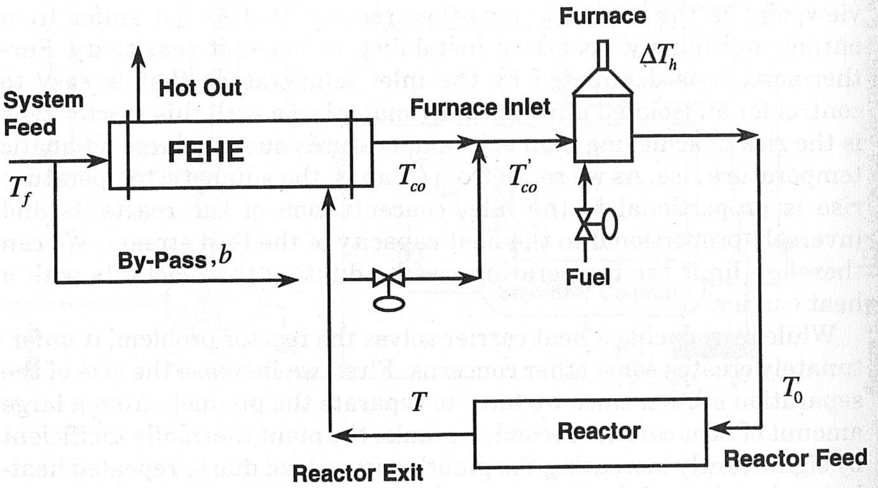


Figure 5.19 Adiabatic plug-flow reactor with feed-effluent heat exchanger and trim heater.

steady states by a graphical technique similar to the one we used for a cooled CSTR in Chap. 4.

We start by plotting the temperature rise in the reactor. This is done by integrating the steady-state differential equations that describe the composition and heat effects as functions of the axial position in the reactor. The adiabatic plug-flow reactor gives a unique exit temperature for a given feed temperature. This also means that we get a unique difference between the exit and feed temperatures. The temperature difference has to be less than or equal to the adiabatic temperature rise at a given, constant feed composition. Figure 5.20 shows the fractional temperature rise as a function of the reactor feed temperature for a typical system.

The next step in the analysis is to seek another functional relationship between the reactor exit temperature and the reactor feed temperature resulting from the heat exchange, bypass, and influence of the furnace. Once we find the second relation we can superimpose it on top of the reactor temperature rise expression shown in Fig. 5.20. Intersections between the two curves constitute open-loop, steady-state solutions to the combined reactor-FEHE system.

Equation (5.5) provides the starting point for our second functional relation. When we use the nomenclature of Fig. 5.19 we get the following simple relationship around the heat exchanger.

$$T_{co} = T_f + \epsilon(T - T_f)$$

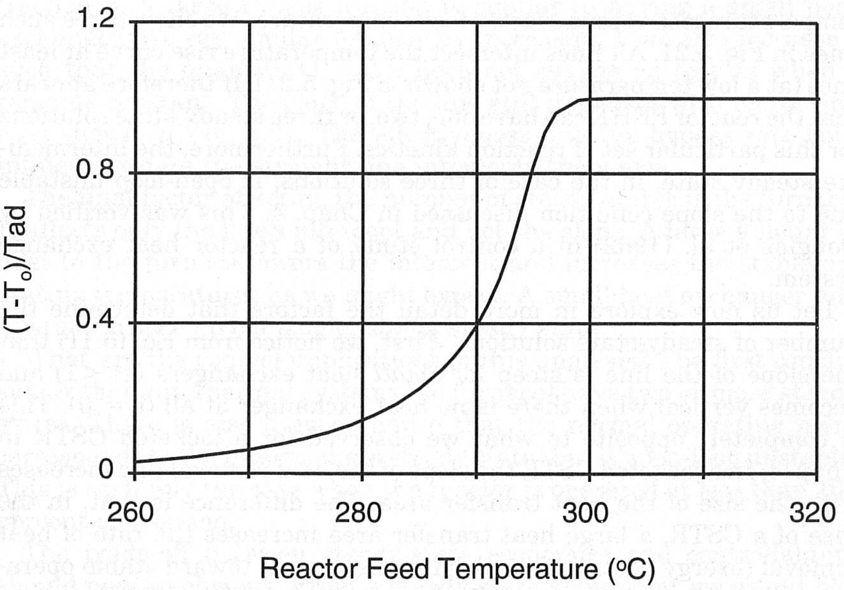


Figure 5.20 Normalized temperature rise in adiabatic plug-flow reactor as function of reactor feed temperature.

This follows since the cold stream to the heat exchanger has the smaller total heat capacity due to the bypass [i.e., $(\dot{m}C_P)_{\min} = (\dot{m}C_P)_C$].

We then add the effect of the bypass as a simple mixing operation:

$$T'_{co} = (1 - b)T_{co} + bT_f$$

where b is the fraction bypass.

The furnace, finally, provides a constant heat input in manual operation. This heat input gives a constant temperature increase ΔT_h. The functional relation between the reactor feed temperature T_0 and the reactor exit temperature T can now be computed:

$$T_0 = (1 - b)[T_f + \epsilon(T - T_f)] + bT_f + \Delta T_h$$

or

$$T = \frac{T_0 + ((1 - b)\epsilon - 1)T_f - \Delta T_h}{(1 - b)\epsilon} \qquad (5.10)$$

By subtracting T_0 from both sides of Eq. (5.10) and dividing by the adiabatic temperature rise ΔT_{ad}, we obtain the following relation:

$$\frac{T - T_0}{\Delta T_{ad}} = \left(\frac{1}{(1 - b)\epsilon} - 1\right) \cdot \frac{T_0 - T_f}{\Delta T_{ad}} - \frac{1}{(1 - b)\epsilon}\frac{\Delta T_h}{\Delta T_{ad}} \qquad (5.11)$$

Equation (5.11) represents a straight line in the diagram of fractional temperature rise versus reactor feed temperature. We show three such lines in Fig. 5.21. All lines intersect the temperature rise curve at least once (at a low temperature not shown in Fig. 5.21). It therefore appears that the reactor FEHE can have one, two, or three steady-state solutions for this particular set of reaction kinetics. Furthermore, the intermediate steady state, in the case of three solutions, is open-loop unstable due to the slope condition discussed in Chap. 4. This was verified by Douglas et al. (1962) in a control study of a reactor heat exchange system.

Let us now explore in more detail the factors that determine the number of steady-state solutions. First, we notice from Eq. (5.11) that the slope of the line is steep for *small* heat exchangers ($\epsilon << 1$) and becomes vertical when there is no heat exchanger at all ($\epsilon = 0$). This is completely opposite to what we observed for a jacketed CSTR in Chap. 4. In a jacketed CSTR the slope of the heat removal line increases with the size of the heat transfer area. The difference is that, in the case of a CSTR, a large heat transfer area increases the rate of heat removal (exergy destruction), driving the system toward stable operation at a single steady state, whereas in the case of an FEHE system,

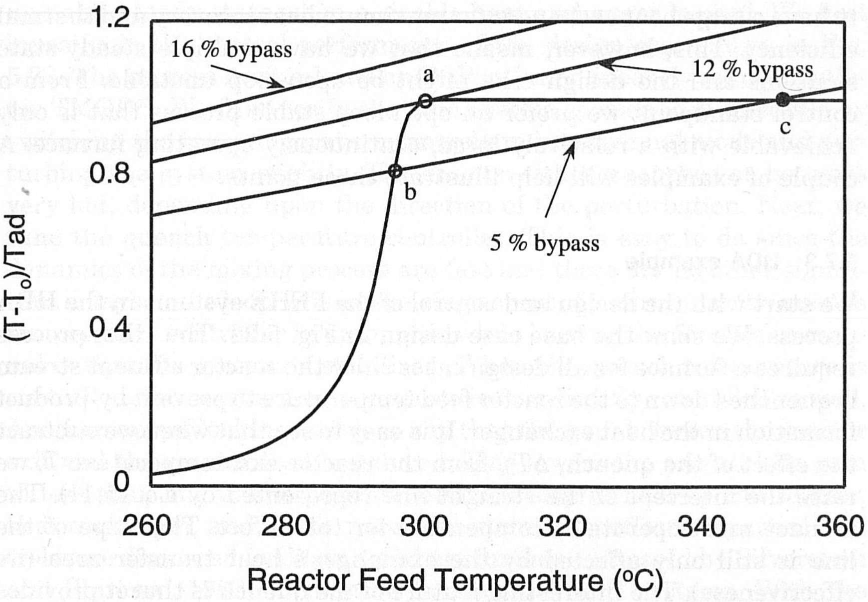


Figure 5.21 Heat removal lines in feed-effluent heat exchange system with bypass.

the large heat transfer area retains heat within the system and thereby promotes the occurrence of multiple solutions.

The second factor affecting the number of steady states is the bypass fraction b. A large bypass fraction is similar to having a small heat exchanger. We say similar because by increasing b we also increase ϵ such that the quantity $(1 - b)\epsilon$ does not change as fast as when ϵ remains constant. The slope of the line still increases with increasing b as shown in Fig. 5.21. The effectiveness and the bypass rate both influence where the straight line intercepts the y axis.

The final factor affecting the number of steady states is the furnace. It affects only the line's intercept and not the slope. A large amount of heat to the furnace lowers the intercept and increases the stable operating temperatures as we might expect. A small heat exchanger and a large furnace give a single, stable steady state.

What are the control implications of this analysis? The first conclusion is that autothermal systems (no furnace) have two or more steady states. There is also a good chance that the normal operating point corresponds to the intermediate steady state that is open-loop unstable. This is certainly the case when the reactor is operated at less than 100 percent conversion.

The trade-off between steady-state economics and controllability should now be obvious. From a steady-state standpoint we would like to have a large heat exchanger for maximum heat recovery and thermal efficiency. This, however, means that we have multiple steady-state solutions and the design case might be open-loop unstable. From a control standpoint we prefer an open-loop stable process that is only achievable with a relatively large, continuously operating furnace. A couple of examples will help illustrate these points.

5.7.3 HDA example

We start with the design and control of the FEHE systems in the HDA process. We show the base case design in Fig. 5.22. The HDA process requires a furnace for all design cases since the reactor effluent stream is quenched down to the reactor feed temperature to prevent by-product formation in the heat exchanger. It is easy to see that when we subtract the effect of the quench, ΔT_q, from the reactor exit temperature T, we raise the intercept of the straight line represented by Eq. (5.11). The furnace must operate to compensate for this effect. The slope of the line is still only affected by the exchanger's heat transfer area (its effectiveness). The interesting feature of the quench is that it provides another manipulated variable that affects the control of the reactor-FEHE system. Since the quench and the furnace have opposing effects on the reactor's feed temperature, we could suspect the possibility of control loop interactions.

The HDA reactor has less than 100 percent per-pass conversion of toluene, meaning that the normal operating point is the intermediate,

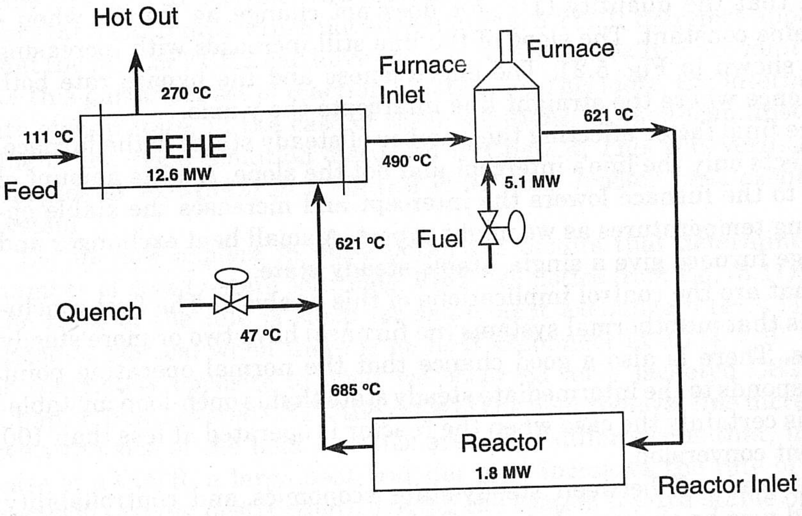


Figure 5.22 HDA process base case process data.

unstable steady state when a sizable heat exchanger is used. We first investigate the control performance of the design case shown in Fig. 5.23. The process is simulated on DuPont's nonlinear dynamic simulator TMODS. We first verify that the system is open-loop unstable by switching the two temperature controllers into manual mode and perturbing the system slightly. The reactor either quenches or becomes very hot, depending upon the direction of the perturbation. Next, we tune the quench temperature controller. This is easy to do since the dynamics of the mixing process are fast and there are no other significant delays in the loop. The interesting aspect of putting just the quench temperature controller in automatic while leaving the furnace in manual is that the system is stabilized. When the quench temperature is controlled, the reactor feed temperature is indirectly controlled as well. Another way of looking at it is to say that the gain between the reactor exit and the reactor feed is reduced. This lowers the overall loop gain to less than one in the positive feedback loop formed by the reactor, heat exchanger, and the furnace. The stabilizing effects of partial control were discussed in Chap. 4 and are further addressed by Silverstein and Shinnar (1982) in relation to reactor-FEHE systems. With the reactor system stabilized it is trivial to tune the reactor feed temperature controller by use of a relay test.

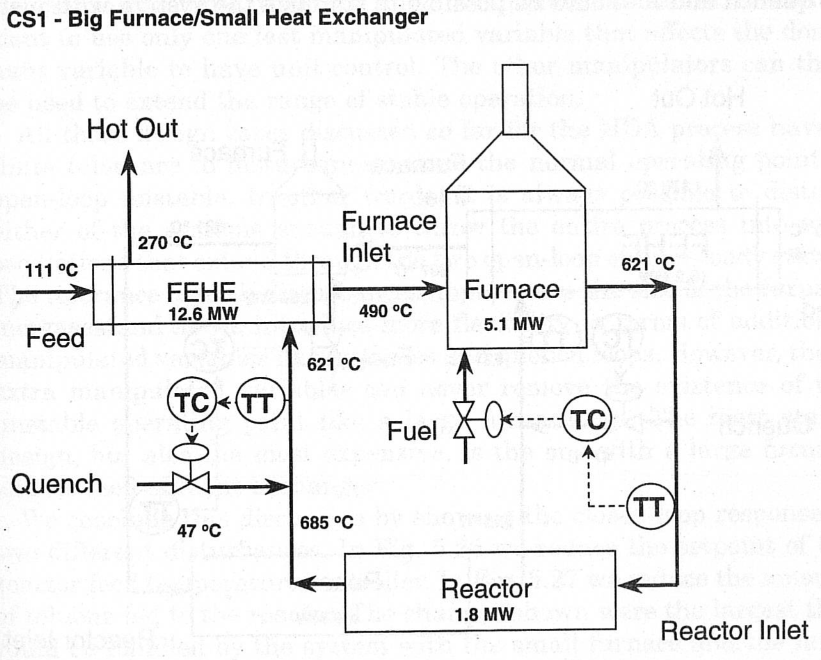


Figure 5.23 HDA process basic heat management control system.

We also tried to stabilize the process by tuning the reactor feed temperature loop while leaving the quench loop in manual. This turned out to be difficult to do since it requires a trial-and-error tuning approach for the open-loop unstable system. However, it was possible to find a combination of gain and reset time that stabilized the system even though it ended up very underdamped. The reason for the difficulties here as opposed to the quench loop is that we assume that the furnace has a much longer time constant than the thermal mixing in the quench loop.

We next try a more aggressive heat recovery alternative as shown in Fig. 5.24. The heat input to the furnace is quite small and most of the heat is provided by the large feed-effluent exchanger. With our choice of measurement lags (two 1-minute lags in series) and the lag in the furnace, this system cannot be stabilized by feedback control around the furnace if the quench controller is in manual. However, it is possible to stabilize the system with just the quench controller in automatic and the furnace controller in manual. Subsequent tuning of the furnace controller is then easy since the new system is open-loop stable.

As we have seen several times in this chapter, a bypass around the heat exchanger introduces another manipulated variable for control. We show such a design in Fig. 5.25. The bypass ought to be as fast as the quench and it should be possible to stabilize the system with just

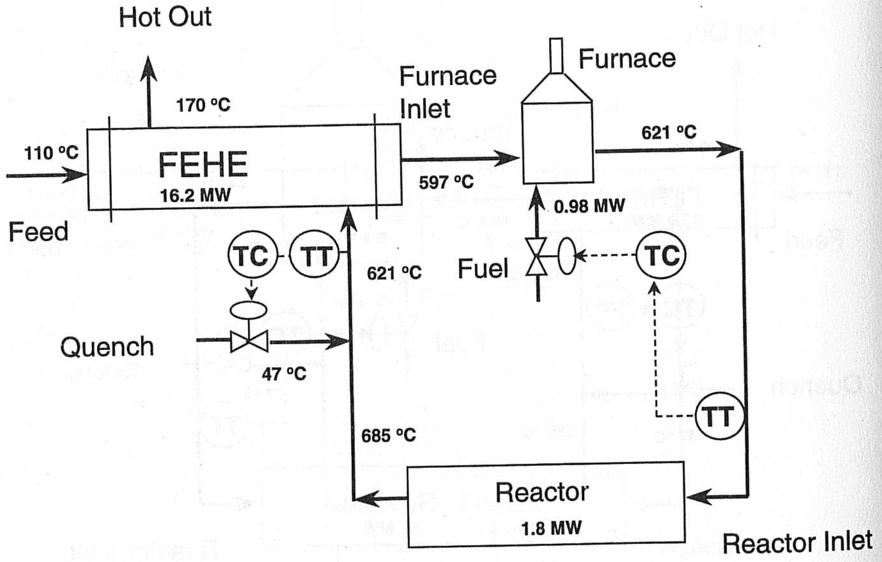


Figure 5.24 HDA process use of large FEHE for maximum heat recovery.

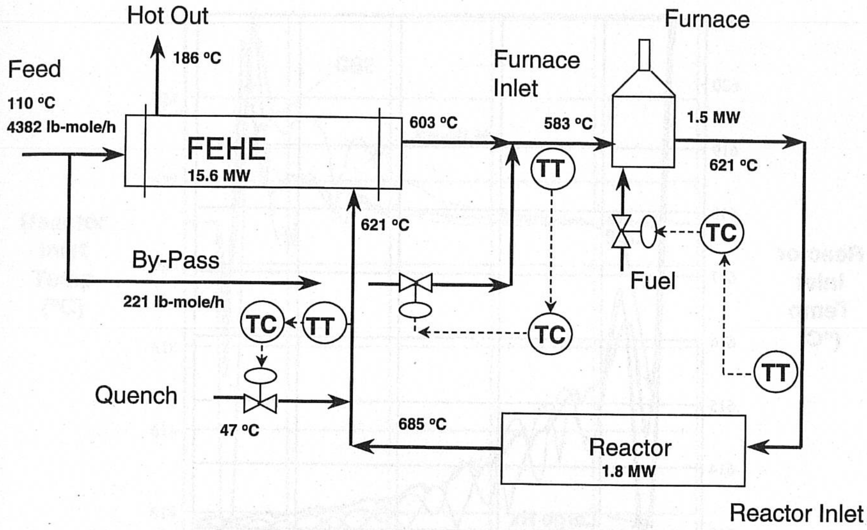


Figure 5.25 HDA process with large FEHE and bypass control.

the bypass loop in automatic. Indeed, we found this to be true. This is a great example of the meaning of partial control discussed in Chap. 4. For the HDA system we happen to have only one dominant variable (reactor inlet temperature) but three manipulated variables. It is sufficient to use only one fast manipulated variable that affects the dominant variable to have unit control. The other manipulators can then be used to extend the range of stable operation.

All three design cases discussed so far for the HDA process have a finite tolerance to disturbances, since the normal operating point is open-loop unstable. In other words, it is always possible to disturb either of the systems enough to throw the entire process into wild oscillations that extend through the two open-loop stable steady states. The tolerance to such disturbances improves as the size of the furnace increases and as we introduce more flexibility in terms of additional manipulated variables like bypasses and quench loops. However, these extra manipulated variables can never remove the existence of the unstable operating point like a large furnace can. The most stable design, but also the most expensive, is the one with a large furnace and no feed-effluent exchanger.

We conclude this discussion by showing the closed-loop response to two different disturbances. In Fig. 5.26 we reduce the setpoint of the reactor feed temperature controller. In Fig. 5.27 we reduce the amount of toluene fed to the reactor. The changes shown were the largest that could be handled by the system with the small furnace and the large exchanger without a bypass. The design with the bypass (CS2) and the

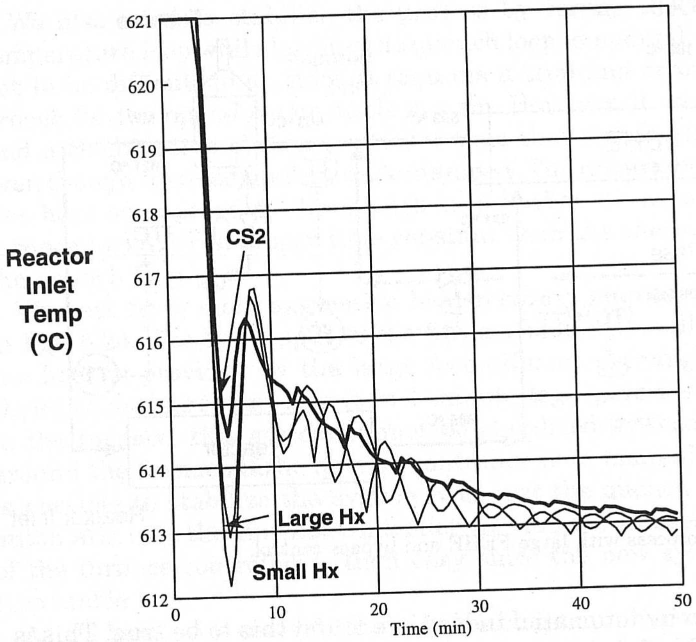


Figure 5.26 Dynamic response of HDA reactor inlet temperature to −8°C setpoint change for three different process and control configurations.

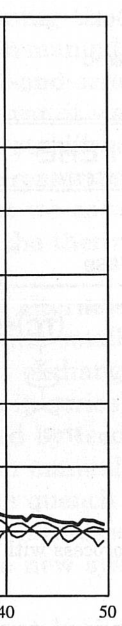
design with the large furnace handle these disturbances quite well and they also tolerate larger upsets than the ones shown here without going unstable.

5.7.4 Reactors with wrong-way behavior

The HDA reactor is unpacked and therefore cannot exhibit the wrong-way behavior discussed in Chap. 4. However, it is quite common that gas phase reactions are carried out over a catalyst so it is important to understand the implications of the wrong-way behavior on the control of reactors with feed-effluent heat exchangers.

To that end we have constructed a simulation of a fictitious system that has a severe inverse response. We show the design in Fig. 5.28 and give the design parameters in Table 5.1. The reactor has a large Lewis number (Le = 25), nearly complete per pass conversion of the reactant, and little axial dispersion. These are all factors necessary for wrong-way behavior. In fact the example plot of wrong-way behavior shown in Chap. 4 was generated from this reactor.

We start by exploring the open-loop characteristics of the autothermal system with a 12 percent bypass rate. We already showed the steady-



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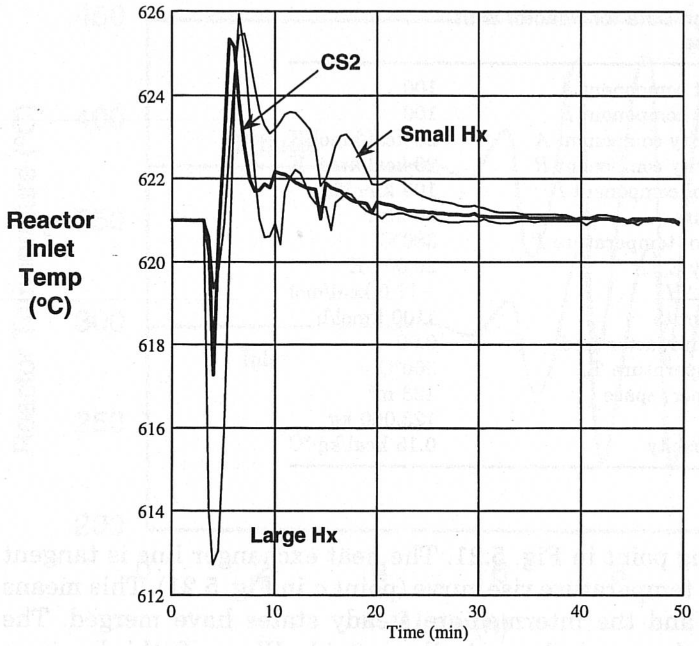

Figure 5.27 Dynamic response of HDA reactor inlet temperature to 15 percent decrease in toluene recycle rate for three different process and control configurations.

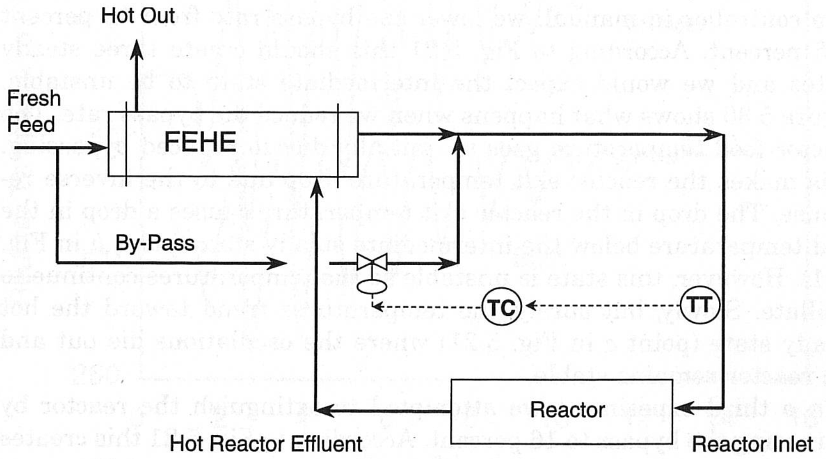

Figure 5.28 Control of packed adiabatic plug-flow reactor with FEHE and bypass control.

TABLE 5.1 Design Data for Reactor with Inverse Response

Molecular weight component *A*	100
Molecular weight component *B*	100
Vapor heat capacity component *A*	20 kcal/kmol·K
Vapor heat capacity component *B*	20 kcal/kmol·K
Production rate of component *B*	100 kmol/h
Operating pressure	15 atm
Reactor design exit temperature T	380°C
Activation energy E_a/R	20,000 K
Heat of reaction ΔH	-17.6 kcal/mol
Reactor feed flowrate	1100 kmol/h
Mole fraction *A* in reactor feed	0.09
Reactor feed temperature T_0	300°C
Reactor void (vapor) space	123 m^3
Packing weight	123,000 kg
Packing heat capacity	0.15 kcal/kg·°C

state operating point in Fig. 5.21. The heat exchanger line is tangent to the reactor temperature rise curve (point *a* in Fig. 5.21). This means that the hot and the intermediate steady states have merged. The combined steady state is dynamically unstable. We verify this by simulating the system shown in Fig. 5.28 with a fixed bypass rate. The results are shown in Fig. 5.29. The bypass valve is held constant from time zero. After about 5 hours of operation, in this mode, the feed and exit temperatures start oscillating. The oscillations grow until the reactor temperatures enter fixed-amplitude-limit cycles.

We next verify that there exists a hot stable steady state when the system equations have three stationary solutions. With the temperature controller in manual, we lower the bypass rate from 12 percent to 5 percent. According to Fig. 5.21 this should create three steady states and we would expect the intermediate state to be unstable. Figure 5.30 shows what happens when we reduce the bypass rate. The reactor feed temperature goes up initially due to reduced bypassing. This makes the reactor exit temperature drop due to the inverse response. The drop in the reactor exit temperature causes a drop in the feed temperature below the intermediate steady state (point *b* in Fig. 5.21). However, this state is unstable so the temperatures continue to oscillate. Slowly, but surely, the temperatures trend toward the hot steady state (point *c* in Fig. 5.21) where the oscillations die out and the reactor remains stable.

In a third experiment we attempted to extinguish the reactor by increasing the bypass to 16 percent. According to Fig. 5.21 this creates a single stable steady state (cold with little or no conversion). However, the result of this experiment, shown in Fig. 5.31, was surprising. Instead of migrating to the cold steady state, the whole system enters into

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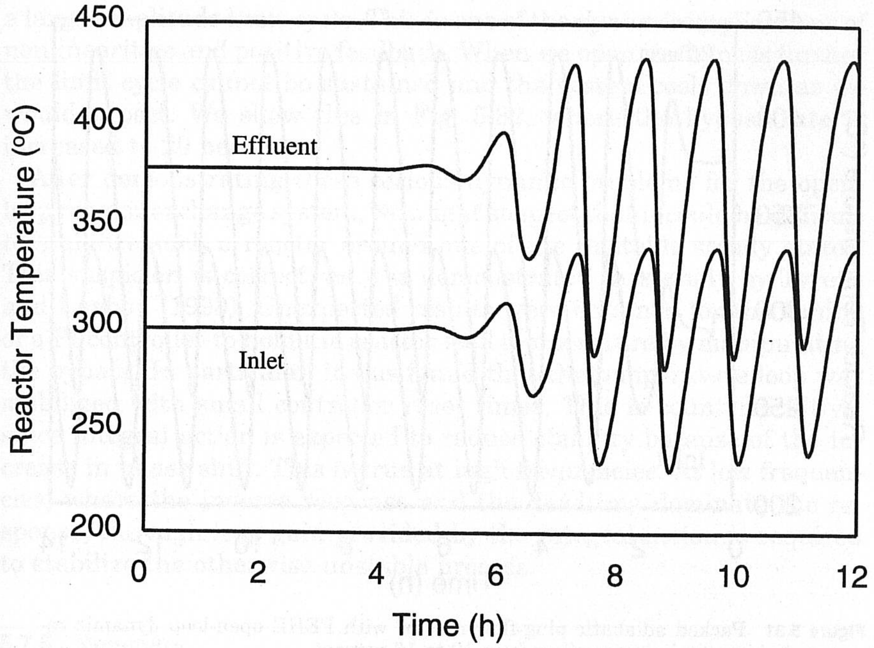


Figure 5.29 Open-loop dynamic behavior of packed adiabatic plug-flow reactor with FEHE.

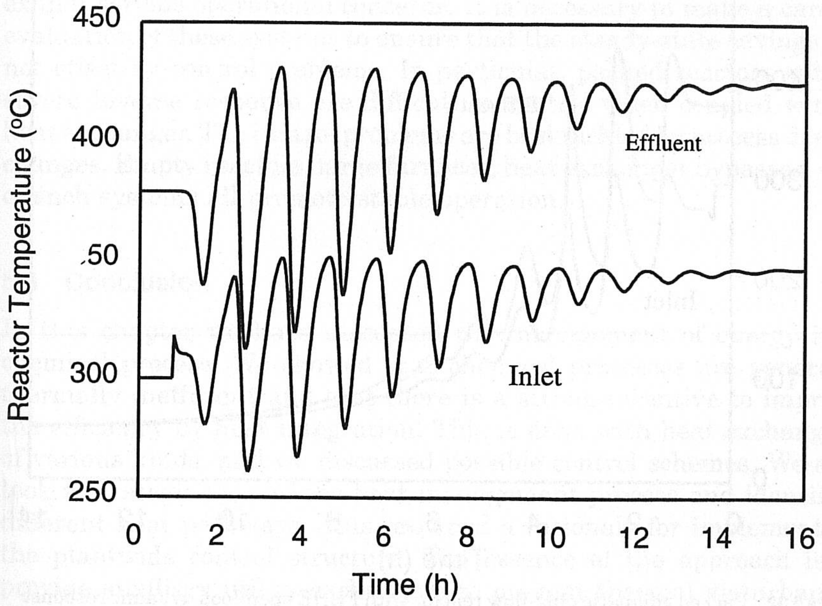


Figure 5.30 Packed adiabatic plug-flow reactor with FEHE open-loop dynamic response to decrease in bypass flow from 12 to 5 percent.

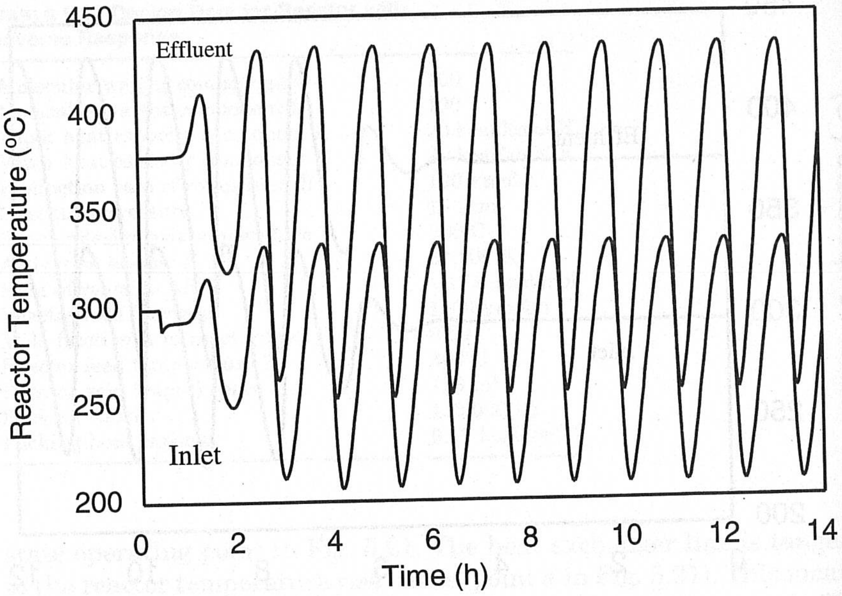


Figure 5.31 Packed adiabatic plug-flow reactor with FEHE open-loop dynamic response to increase in bypass flow from 12 to 16 percent.

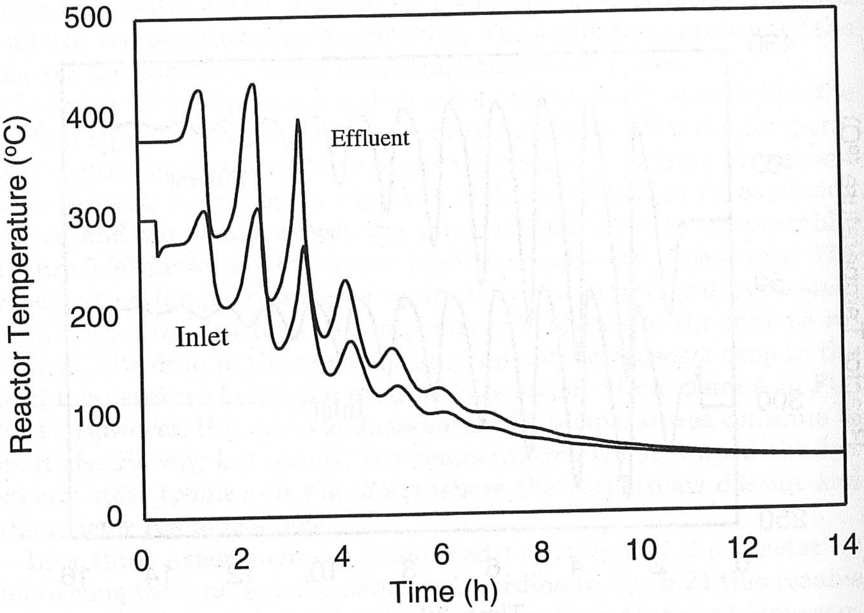
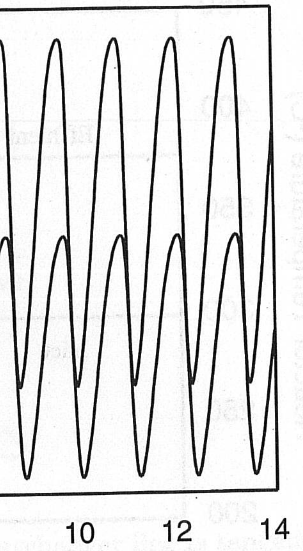


Figure 5.32 Packed adiabatic plug-flow reactor with FEHE open-loop dynamic response to increase in bypass flow from 12 to 20 percent.



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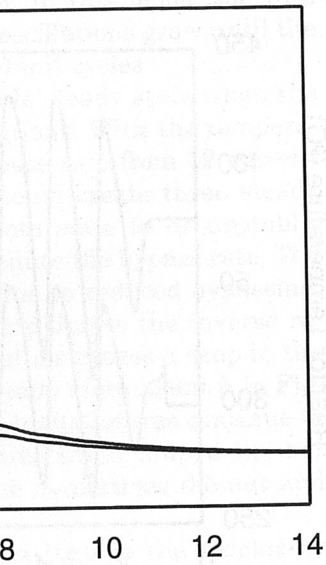

EHE open-loop dynamic response

a large-amplitude limit cycle. This is one of the *dynamic* implications of nonlinearities and positive feedback. When we open the bypass further the limit cycle cannot be sustained and the system cools down as we would expect. We show this in Fig. 5.32, where the bypass rate is increased to 20 percent.

After demonstrating these serious dynamic problems for the open-loop reactor exchange system, we might suspect that it could be difficult to stabilize such a reactor around one of the unstable steady states. This suspicion is correct, as was demonstrated in a study by Tyreus and Luyben (1993). Unexpected results were obtained for the tuning of a PI controller to hold the reactor feed temperature by manipulating the bypass. In particular, it was found that the temperature loop was stabilized with small controller reset times. This is counterintuitive, since integral action is expected to reduce stability because of the increase in phase shift. This is true at high frequencies. At low frequencies, where the inverse response and the deadtime dominate the response, the high loop gain provided by the integral action is required to stabilize the otherwise unstable process.

5.7.5 Summary

We have discussed in detail the design, open-loop behavior, and control of adiabatic, plug-flow reactors with feed-effluent exchangers. These systems are attractive from a steady-state economic viewpoint but can exhibit serious operational concerns. It is necessary to make a careful evaluation of these systems to ensure that the steady-state savings are not offset by control problems. In particular, packed reactors with a severe inverse response are difficult to control when coupled with a heat exchanger. The control problems are best tackled by process design changes. Empty reactors, large furnaces, heat exchanger bypasses, and quench systems all promote stable operation.

5.8 Conclusion

In this chapter we have discussed the management of energy in a chemical process. We showed that chemical processes are generally thermally inefficient and that there is a strong incentive to improve the efficiency by heat integration. This is done with heat exchangers of various kinds, and we discussed possible control schemes. We also took a strategic view of the heat management process and identified different heat pathways. This provided a rationale for implementing the plantwide control structure. The essence of the approach is to provide auxiliary utility exchangers to prevent thermal disturbances from propagating through the plant. Since these auxiliary exchangers can add significantly to the cost of the plant, we indicated that more cost-effective designs merely involve reactor feed-effluent heat exchangers. The dynamics and control of these systems were discussed in detail. We found that the most stable systems include a large furnace and bypasses around the feed-effluent exchangers.

5.9 References

Douglas, J. M., Orcutt, J. C., and Berthiaume, P. W. "Design and Control of Feed-Effluent, Exchanger-Reactor Systems," *Ind. Eng. Chem. Fundam.*, **1,** 253–257 (1962).

Douglas, J. M. *Conceptual Design of Chemical Processes*, New York: McGraw-Hill (1988).

Gebhart, B. *Heat Transfer,* 2d ed., New York: McGraw-Hill (1971).

Handogo, R., and Luyben, W. L. "Design and Control of a Heat-Integrated Reactor/Column Process," *Ind. Eng. Chem. Res.,* **26,** 531–538 (1987).

Jones, W. E., and Wilson, J. A. "An Introduction to Process Flexibility. 1. Heat Exchange," *Chemical Engineering Education*, **31,** 172–177, Summer (1997).

Silverstein, J. L., and Shinnar, R. "Effect of Design on the Stability and Control of Fixed Bed Catalytic Reactors with Heat Feedback. 1. Concepts," *Ind. Eng. Chem. Proc. Des. Dev.*, **21,** 241–256 (1982).

Terrill, D. L., and Douglas, J. M. "A *T-H* Method for Heat Exchanger Network Synthesis," *Ind. Eng. Chem. Res.*, **26,** 175–179 (1987a).

Terrill, D. L., and Douglas, J. M. "Heat-Exchanger Network Analysis. 1. Optimization," *Ind. Eng. Chem. Res.*, **26,** 685–691 (1987b).

Terrill, D. L., and Douglas, J. M. "Heat-Exchanger Network Analysis. 2. Steady-State Operability Evaluation," *Ind. Eng. Chem. Res.*, **26,** 691–696 (1987c).

Tyreus, B. D., and Luyben, W. L. "Controlling Heat Integrated Distillation Columns," *Chem. Eng. Prog.*, **72,** No. 9, 59–66 (1976).

Tyreus, B. D., and Luyben, W. L. "Unusual Dynamics of a Reactor/Preheater Process with Deadtime, Inverse Response and Openloop Instability," *J. Proc. Cont.*, **3,** 241–251, (1993).