CHAPTER IV

PROCESS AND DESIGN

4.1 Introduction

As discussed in the previous chapter, a network will be resilient if disturbance loads can be transferred to heaters or coolers in order to maintain target temperatures at the specified values. Furthermore, this action should not violate MER, i.e. disturbance entering or originating in a hot side should be transferred to heater and similarly disturbances entering or originating in a cold side should be dissipated in coolers. Since the variations in inlet temperatures and flowrates cause changes in pinch temperature location, the determination of where disturbances should be destined at any particular time is a control problem.

Hence, the design problem is not only to provide a path in a network for the specified disturbance to be transmitted to heaters and coolers but also to generate a structure that can handle the pinch relocation, i.e. redirection the disturbances to appropriate heat sinks or heat sources according to the disturbances. In this research, the design strategy for the pinch move is applied. The *pinch-defined region* is specified by the maximum and minimum values of the pinch temperatures. The problem is divided into a hot side and a cold side. However the hot side pinch temperature is the maximum and the process streams are attached with uncertain heat loads according to pinch temperature variation. Thus, for a hot stream, the maximum outlet temperature is the maximum pinch whereas the minimum outlet temperature is the minimum pinch. The partitioning procedure of a cold side is similar. The cold side pinch temperature is the minimum pinch and the pinch temperature of the process streams in the cold side as in the hot side are subjected to variations according to temperature. By this strategy, a new disturbance is created in the pinch region for those streams which cross the pinch zone. The synthesis procedure must account both inlet and pinch-induced disturbances.

4.2 The Synthesis Procedure

The synthesis of a resilient heat exchanger network by using (1) match patterns as operators in mapping one design state to the next and (2) heat load propagation technique can be done by the following systematic sequence:

1. Pop a match pattern operator from the ordered stack of match patterns. If all the patterns are chosen backtrack to the parent designed state and repeat the procedure. If the current state is the starting state and all patterns have been tried without success the problem cannot be solved with the current knowledge in the rule –based system. A trade-off between cost and resiliency may be needed.

2. Choose a pair of hot and cold streams from the set of unmatched process streams. If all the streams have been chosen and none were satisfied, go back to the first step to try a new pattern.

3. Apply the match pattern to the selected pair of streams. If the streams satisfy the pattern test and the resiliency requirement, go to the next step. Otherwise go back to the previous step to select a new pair of streams.

Match pattern test: Check whether the heat load, input temperatures and heat flowrate capacity satisfy the match pattern description.

Resiliency test: Check whether the disturbance load of the smaller heat load stream can be shifted to the larger heat load stream.

4. Create a new state to support the new fact. A new state is a descendant of a current one. Change the parameters of the larger heat load stream: the supply or target temperature, the heat load the disturbance load.

The new supply or target temperature will be adjusted according to the regular heat load and the disturbance heat load of the matched stream.
The new heat load of the residual streams is the value between the supply and target temperatures at the design condition.

The new disturbance load is the sum of the disturbance load of both matched streams. A special treatment is needed for a pinch match or the match starts off from the pinch point. The new disturbance will be the sum of the upstream disturbance of a stream in the match pair and the difference between the pinch included disturbance of the two streams. See Figure 4.1.

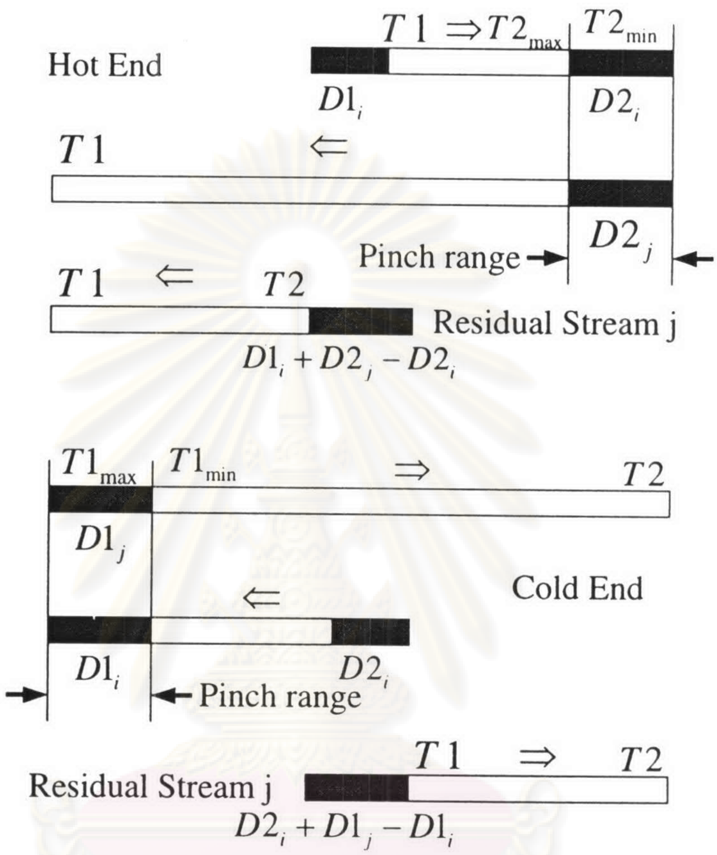


Figure 4.1 A Pinch Match on the Propagated Disturbance Concept

For a pinch match of streams i and j for which $W_j > W_i$ and $L_j > L_i$ the disturbance of a residual stream:

$$D_j = D_i + (D_{j\,pinch} - D_{i\,pinch})$$

The disturbance at the pinch of the two streams must be deductive instead of being additive as in general case. Since the variations of the inlet temperature of stream j and outlet temperature of stream I are not independently varied but tied to the pinch temperature.

The disturbance at outlet stream position include by the pinch variation has no net effect to the other streams since:

o By the deductive effect described above. It should be noted here that by considering only match pattern Class A and Class B, only a larger heat load and heat capacity flowrate stream can be matched to such a stream. Therefore its downstream disturbance will be engulfed by a larger stream to which such a stream is matched. Only the remaining upstream disturbance of a small stream (if there is any), will be propagated to its own residual stream.

o No none-pinched stream can be matched to such stream because of the temperature constraint.

5. If there are unmatched hot and cold streams, go to the second step. Otherwise go to the next step.

6. Match the only hot or cold streams with the utility streams.

7. If there are other unused match patterns go to the first step. This is equivalent to saying that there might be other solutions available, continue.

4.3 The Resilience Index, (RI)

We first present a simple procedure to determine the RI for network structures with specified ΔT_{min}. It is based on the "Temperature Interval" method (Linnhoff and flower, 1978) and "Pinch Design" method (Linnhoff and Hindmarsh, 1982). A similar approach was used recently by Snyder (1982) to synthesize resilient HENs.

The idea is following:

We start with the feasible network structure for nominal conditions. The disturbance load on each stream i is represented by an equivalent fictitious heater or cooler with variable load l_i. These heaters and coolers are shifted through the heat exchangers and merged with the heater(s) and cooler(s) originally present in the network. This changes the loads and approach temperatures in the exchangers. The condition for a network structure to be resilient with respect to these disturbances is that after all the disturbance heaters and coolers have been shifted. The load is non-negative and the ΔT_{min} constraint is satisfied for every exchanger.

Linnhoff and Hindmarsh (1982) showed that for a network featuring MER no heat is transferred across the pinch point. This implies that in order to preserve MER the disturbance heaters and coolers must not be shifted across the pinch but only within the "heater section" and the "cooler section".

The "shift-approach " is not very convenient when several disturbances have to be considered simultaneously as in the case for the computation of the RI. In order to simplify the investigation of the changes in exchanger loads L and approach temperatures caused by disturbance load shifts we define a resilience parameter R for each exchanger in the HEN:

$$R = w_s(\Delta T_s - \Delta T_{min})$$

Where w_s is the smaller one of the heat capacity flow rates of the two streams and ΔT_s is the smaller one of the ΔT values at the two ends of the exchanger. R has the same physical dimension as a heat load. The ΔT_m constraint requires R always to be non-negative.

The changes $\Delta R, \Delta L$ caused by a load shift are listed in Table 4.1. It can be seen that the magnitude of these changes is always less than or equal to the load l which is shifted, i.e.

$$\Delta R,\ \Delta L < l\ *$$

Let L_0, R_0 be the load and resilience parameter of and exchanger at the nominal operating point. After a load " l " is shifted though that exchanger, the approach temperature and positive load constraints require that

$$R \geq R_0 - \Delta R \geq 0$$

and

$$L \geq L_0 - \Delta L \geq 0\ **$$

From (*) we conclude that a sufficient condition for (**) to be satisfied is

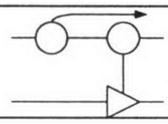
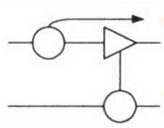
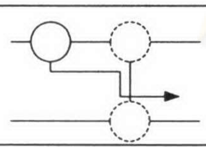
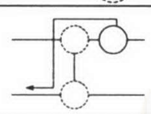
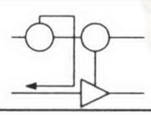
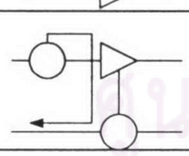
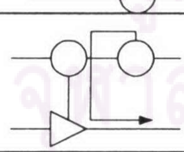
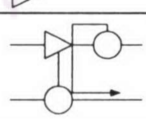
$$L \leq R_0 \text{ and } l \leq L_0$$

Therefore the largest load l_{max} which can be shifted through an exchanger is

$$L_{max} = min\ (L_0, R_0)$$

For a pinch exchanger is always Zero and does not change with load shifts, i.e. (see Table 4.1) Therefore for pinch exchangers, By definition, the RI is equal to the largest arbitrary disturbance load which can be shifted through every exchanger in the network structure without making any exchanger load or resilience parameter negative. Therefore, the RI for the network is the network is the smallest of the determined for the individual exchangers in the network.

Table 4.1 Effect of load shifts on the load and resilience parameter of and exchanger (The triangle indicates the stream with the larger capacity flowrate. It is pointed the side with the smaller ΔT)

Mode of load shift	Effect on ΔR	Effect on ΔL
	l	0
	$l\left(\frac{w_S}{w_L}\right)$	0
	$l\left(\frac{w_S}{w_L}\right)$	l
	l	l
	0	l
	$l\left(1-\frac{w_S}{w_L}\right)$	l
	$l\left(1-\frac{w_S}{w_L}\right)$	l
	0	l

Based on this analysis a simple procedure to determine an estimate of the RI and the maximum variations in stream inlet temperatures can be stated:

Procedure

(1) For every non-pinch exchanger "i" in the network, calculate at the nominal operating point

$$l_{imax} = min\{L_0, R_0\}$$

(2) For every pinch exchanger, heather or cooler "i", in the network, calculate at the nominal operating point

$$l_{imax} = \{L_0\}$$

(3) The RI for the network structure is estimated as

$$RI \geq min\ \{l_{ima}\}$$

According to the definition of the RI the starting temperature variations are bounded by

$$\sum_i \alpha_i \left|T_i^S\right| \leq RI$$

Where

$$\alpha_i = \max\left\{\sum_{j\in P.E.}^{H.S.} w_{L_j}, \sum_{j\in P.E}^{C.S} w_{L_j}\right\}$$

If T_i^s is the pinch point

otherwise $\alpha_i = w_i$

Here $\sum_{j\in P.E.}^{H.S.} w_{L_j}$ and $\sum_{j\in P.E.}^{C.S.} w_{L_j}$ are the sum of the larger heat capacity flow rates in all the pinch exchangers in the "heater " and " cooler " section respectively. This correction for changed in the pinch temperature is necessary because its variations not only affect stream I but also all the other streams at the pinch point. If only one inlet temperature varies and the others remain constant, its maximum allowed variation is given by

$$\left|\Delta T_i^S\right| \leq \frac{RI}{\alpha_i}$$

4.4 The Hydrodealylation Process, (HDA Process)

In this section, we presented the process for the Hydrodealkylation (HDA) which convert toluene to produced benzene. Figure 4.2 shows the nine basic unit operations of the HDA process as described in Douglas (1988): reactor, furnace, vapor-liquid separator, recycle compressor, two heat exchangers, and there distillation columns. Two raw materials, hydrogen and toluene, are converted into the benzene product, with methane and diphenyl produced as by-products. The two vapor-phase reaction are:

$$Toluene + H_2 \longrightarrow Benzene + CH_4$$

$$2Benzene \rightleftharpoons Diphenyl + H_2$$

The kinetic rate expressions are functions of the partial pressures (in psia). The toluene p_T, hydrogen p_H, benzene p_B, and diphenyl p_D, with an Arrhenius temperature dependence. Zimmerman and York (1964) provided the following rate expressions:

$$r_1 = 3.6858\times10^6 \exp(-25{,}616/T)\, p_T\, p_H^{1/2}$$

$$r_2 = 5.987\times10^4 ep(-25{,}616/T)\, p_B^2 - 2.553\times10^5 \exp(25{,}616/T)\, p_D\, p_H$$

where r_1, and r_2 have units of lb-mol/min.ft^3 and T is the absolute temperature in Kelvin. The heats of reaction given by Douglas (1988) are –21,500 Btu/lb-mol of toluene for r_1 and 0 Btu/lb-mol for r_2

The effluent from the adiabatic reactor is quenched with liquid from the separator. This quenched stream is the hot-side feed to the process-to-process heat exchanger, where the cold stream is the reactor feed stream prior to the furnace. The reactor effluent is then cooled with cooling water, and the vapor (hydrogen, methane) and liquid (benzene, toluene, diphenyl) are separated. The vapor stream from the separator is split. Part is purged from the process to remove the methane by-product and the remainder is sent to the compressor for recycle back to the reaction.

The liquid stream from the separator (after part is taken for the quench) is fed to stabilizer column, which has a partial condenser and removes any remaining hydrogen and methane gas from the liquid components. The bottoms stream from the stabilizer is fed to the product column, where the distillate is the benzene product from the process and the bottoms is toluene and diphenyl fed to the recycle column. The distillate from the recycle column is toluene that is recycled back to the reactor and the bottom is the diphenyl byproduct.

Makeup toluene liquid and hydrogen gases are added to both the gas and toluene recycle streams. This combined stream is the cold-side feed to the process-to-process heat exchanger. The cold-side exit stream is then heated further up to the required reactor inlet temperature in the furnace, where heat is supplied via combustion of fuel.

Pure component physical property data for the five species in our simulation of the HDA process were obtained from Chemical Engineering (1975) (liquid densities, heat capacities, vapor pressures, etc.). Vapor-liquid equilibrium behavior was assumed to be ideal. Much of the flow sheet and equipment design information was extracted from Douglass (1988). We have also determined certain design and control variables (e.g., column feed location, temperature control trays, over head receiver and column base liquid holdups) that are not specified by Douglas. Tables 4.2 to 4.5 contain data for selected process streams. These data come from our TMODS dynamic simulation and not from a commercial steady-state simulation package. The corresponding stream numbers are shown in Fig. 4.2 our simulation, the stabilizer column is modeled as a component as a splitter and tank. A heater is used to raise the temperature of the liquid feed stream to the product column. Table 4.6 presents equipment data and Table 4.7 compiles the heat transfer rates within process equipment.

Table 4.2 Process Stream Data, Part 1

	Fresh toluene	Fresh hydrogen	Purge gas	Stabilizer gas	Benzene product	Diphenyl product
Stream number	1	2	3	4	5	6
Flow, lb-mol/h	290.86	490.38	480.88	21.05	272.5	6.759
Temperature, °F	86	86	115	113	211	559
Pressure, psia	575	575	480	480	30	31
H_2,mole fraction	0	0.97	0.3992	0	0	0
CH_4	0	0.03	0.5937	0.9349	0	0
C_6H_6	0	0	0.0065	0.0651	0.9997	0
C_7H_8	1	0	0.0006	0	0.0003	0.00026
$C_{12}H_{10}$	0	0	0	0	0	0.99974

Table 4.3 Process Stream Data, Part 2

	Gas recycle	Toluene recycle	Furnace inlet	Reactor inlet	Reactor effluent	Quench
Stream number	7	8	9	10	11	12
Flow, lb-mol/h	3519.2	82.14	4382.5	4382.5	4382.5	156.02
Temperature, °F	115	272	1106	1150	1263.2	113
Pressure, psia	513	30	513	503	486	486
H_2,mole fraction	0.3992	0	0.4291	0.4291	0.3644	0
CH_4	0.5937	0	0.4800	0.4800	0.5463	0.0515
C_6H_6	0.0065	0.00061	0.0053	0.0053	0.0685	0.7159
C_7H_8	0.0006	0.99937	0.0856	0.0856	0.0193	0.2149
$C_{12}H_{10}$	0	0.00002	0	0	0.0015	0.0177

Table 4.4 Process Stream Data, Part 3

	FEHE hot in	FEHE hot out	Separator gas out	Stabilizer feed	Stabilizer bottoms	Product bottoms
Stream number	13	14	15	16	17	18
Flow, lb-mol/h	4538.5	4538.5	4156.0	382.5	361.4	88.91
Temperature, °F	1150	337	113	113	200*	283
Pressure, psia	486	480	486	480	480	33
H_2,mole fraction	0.3518	0.3518	0.3992	0	0	0
CH_4	0.5294	0.5294	0.5937	0.0515	0	0
C_6H_6	0.0907	0.0907	0.0065	0.7159	0.7538	0.0006
C_7H_8	0.0260	0.0260	0.0006	0.2149	0.2275	0.9234
$C_{12}H_{10}$	0.0021	0.0021	0	0.0177	0.0187	0.0760

*Stream temperature not based upon bubble point but set by heater.

Table 4.5 Process Stream Data, Part 4

	Product column reflux	Recycle column reflux
Stream number	19	20
Flow, lb-mol/h	300	12.0
Temperature, °F	211	272
Pressure, psia	30	30
H_2,mole fraction	0	0
CH_4	0	0
C_6H_6	0.9997	0.00061
C_7H_8	0.0003	0.99937
$C_{12}H_{10}$	0	0.00002

Table 4.6 Equipment Data and Specifications

Reactor	Diameter	9.53 ft
FEHE	Length	57 ft
	Area	30000 ft^2
Furnace	Shell volume	500 ft^3
Separator	Tube volume	500 ft^3
	Tube volume	300 ft^3
	Liquid volume	40 ft^3
Product column	Total theoretical trays	27
	Feed tray	15
	Diameter	5 ft
	Theoretical tray holdup	2.1 lb-mol
	Efficiency	50%
	Reflux drum liquid holdup	25 ft^3
	Column base liquid holdup	30 ft^3
Recycle column	Total theoretical trays	7
	Feed tray	5
	Diameter	3 ft
	Theoretical tray holdup	1 lb-mol
	Efficiency	30%
	Reflux drum liquid holdup	100%
	Column base liquid holdup	15 ft^3

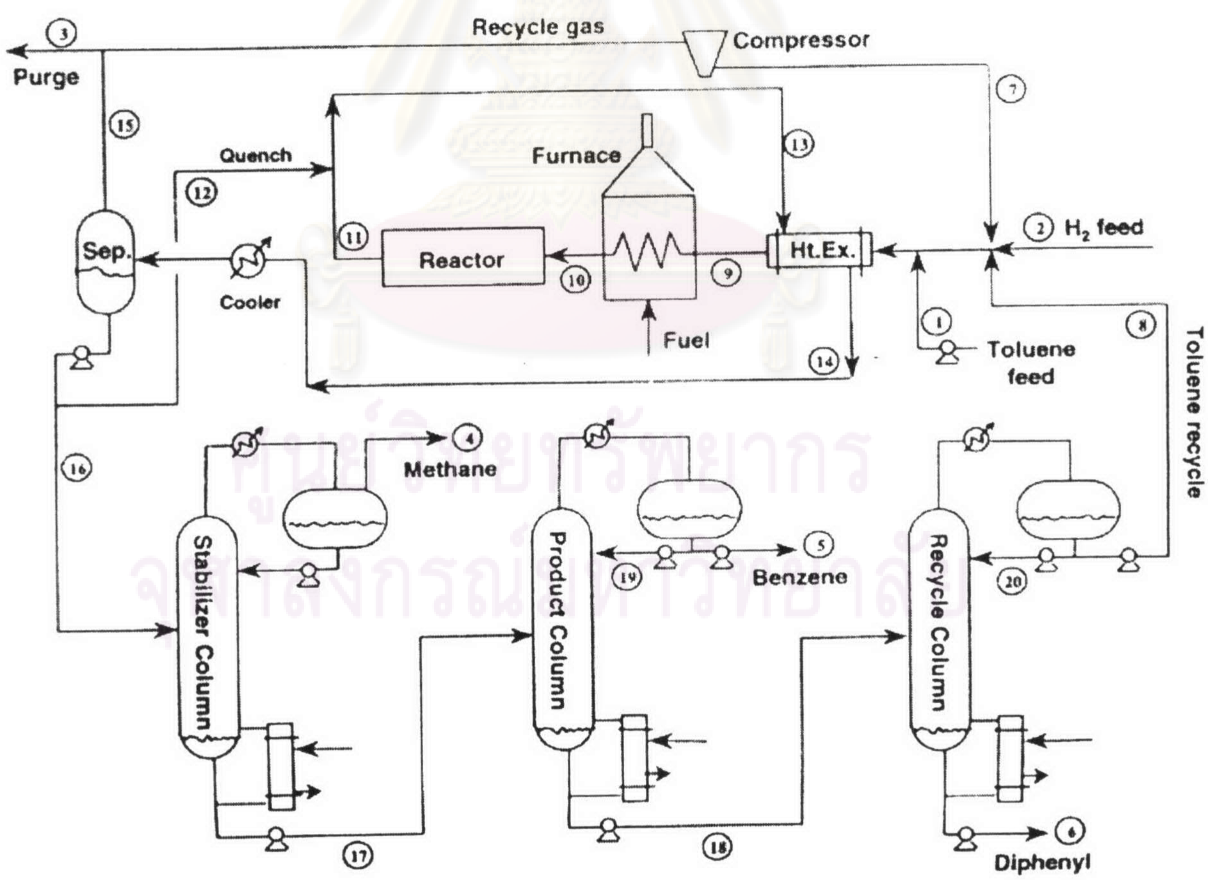


Figure 4.2 HDA Process Flowsheet

Table 4.7 Heat Transfer Rates

FEHE	19.4 MW
Funace	0.984 MW
Separator condenser	5.47 MW
Product reboiler	2.18 MW
Product condenser	2.05 MW
Recycle reboiler	0.439 MW
Recycle condenser	0.405 MW
Reactor heat generation	1.83 MW

4.5 The HDA Alternatives

A study of the sensitivity of the total processing costs to heat-exchanger network alternatives was undertaken by Terrill and Douglas. They developed a heat-exchanger network, for a base-case design (x=0.75, y_{pH}=0.4) for the HDA process. The T-H diagram is shown in Fig.8.10-1. They also developed six alternative heat-exchanger networks, all of which had close to the maximum energy recovery (see Figure 4.3 through 4.8). (Note that the quench stream after the reactor is not shown on these graphs.) Most of the alternatives include a pressure shifting of the recycle column, and the other distinguishing feature is the number of column reboilers that are driven by the hot reactor products.

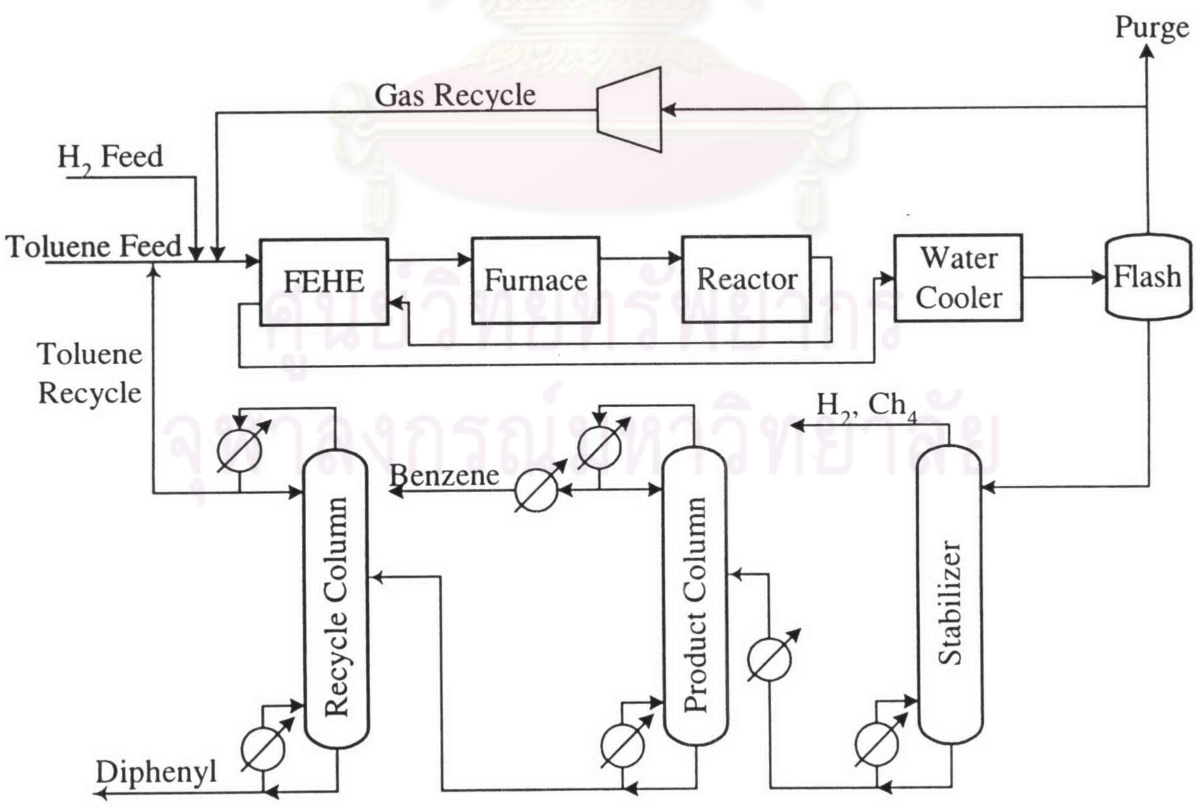


Figure 4.3 Alternative 1 For the HDA Process

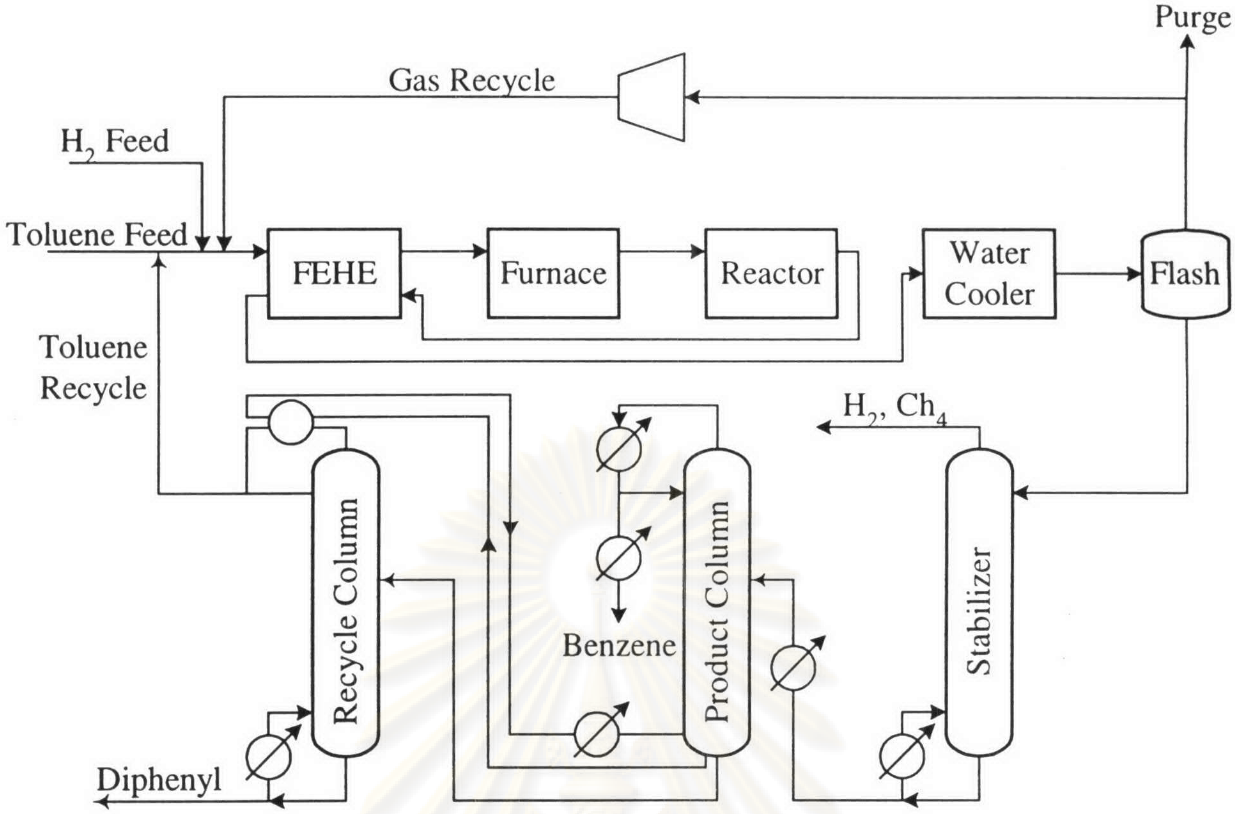


Figure 4.4 Alternative 2 For the HDA Process

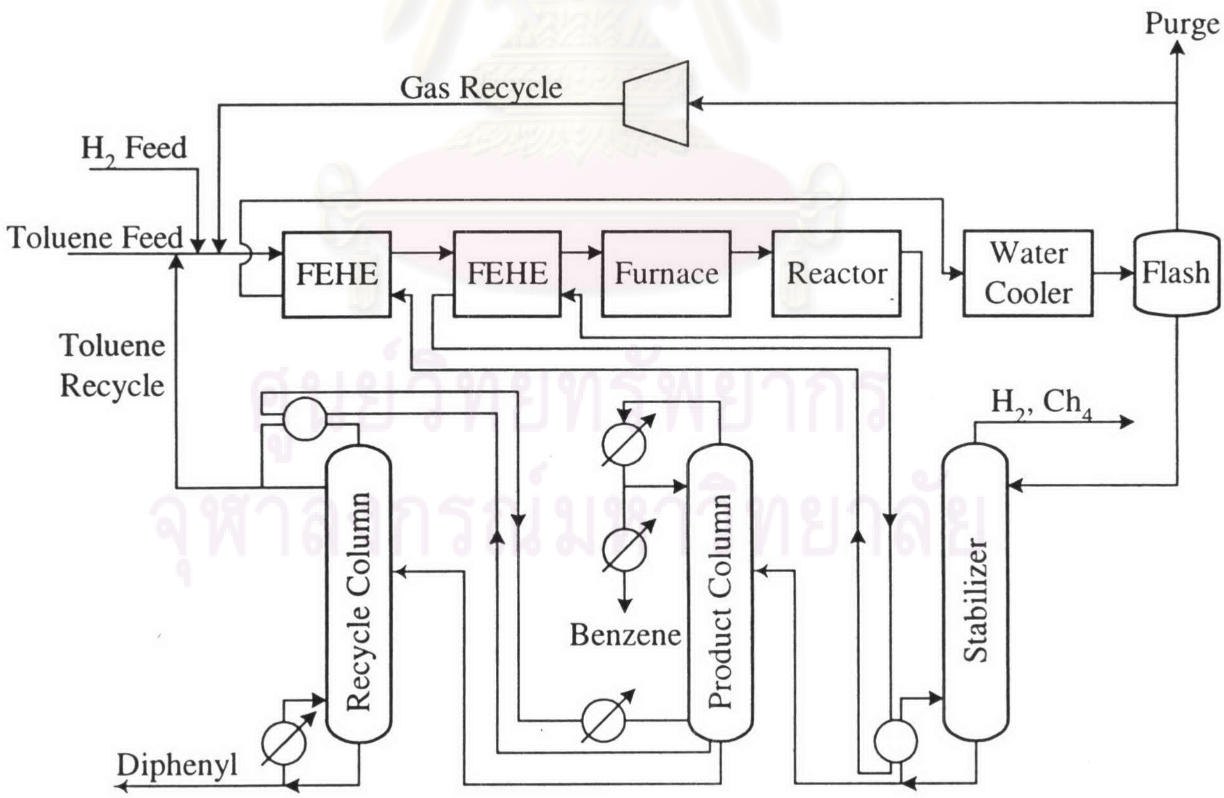


Figure 4.5 Alternative 3 For the HDA Process

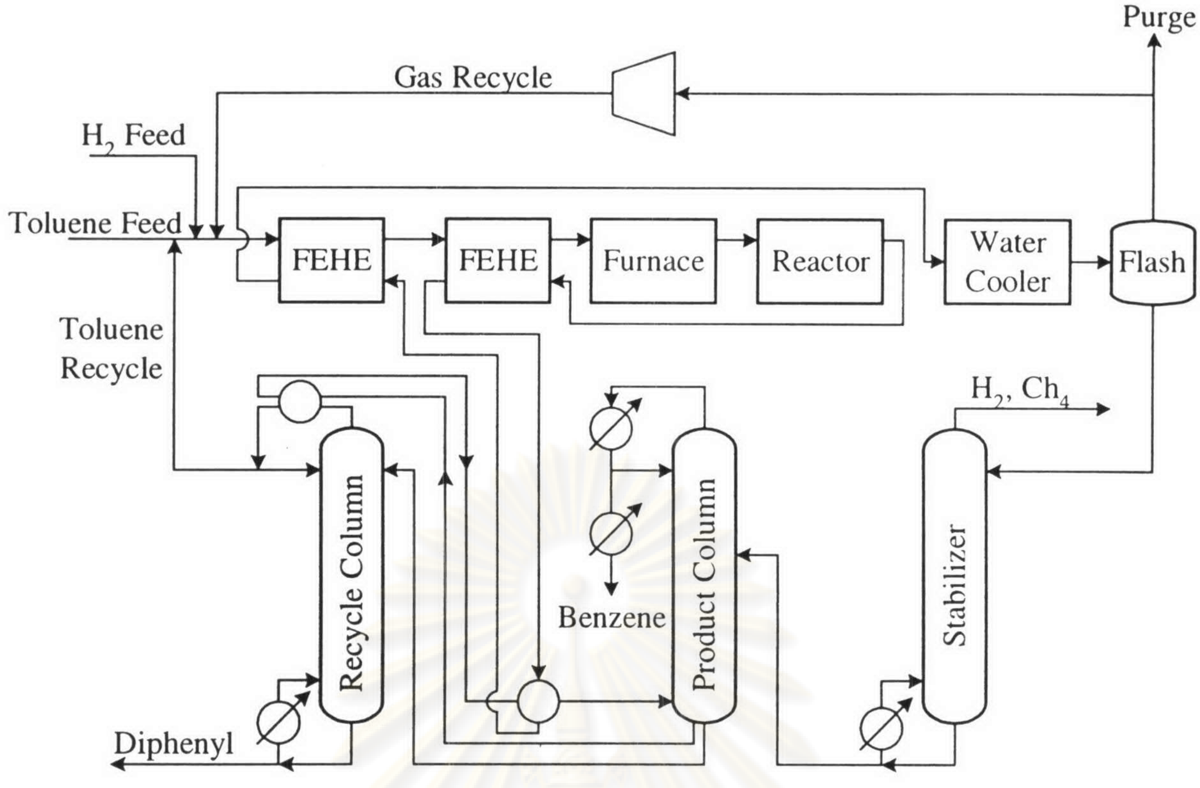


Figure 4.6 Alternative 4 For the HDA Process

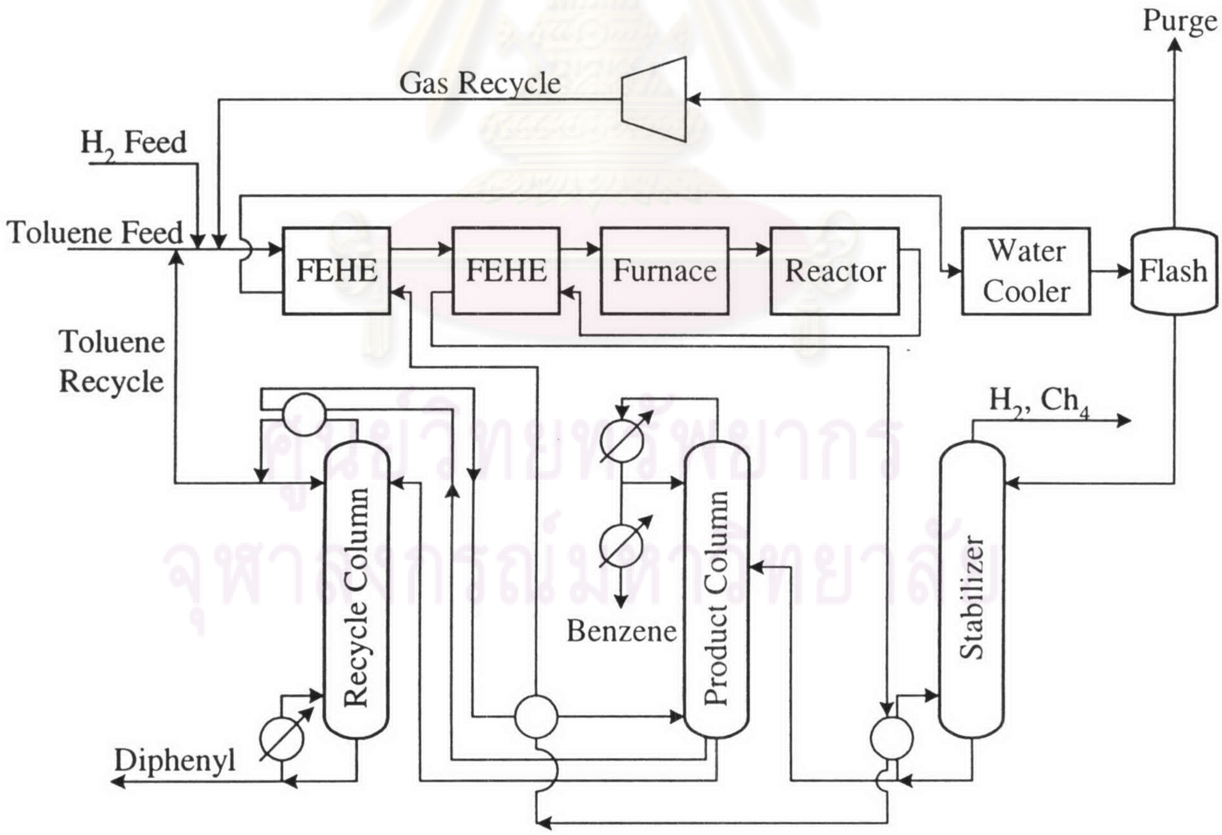


Figure 4.7 Alternative 5 For the HDA Process

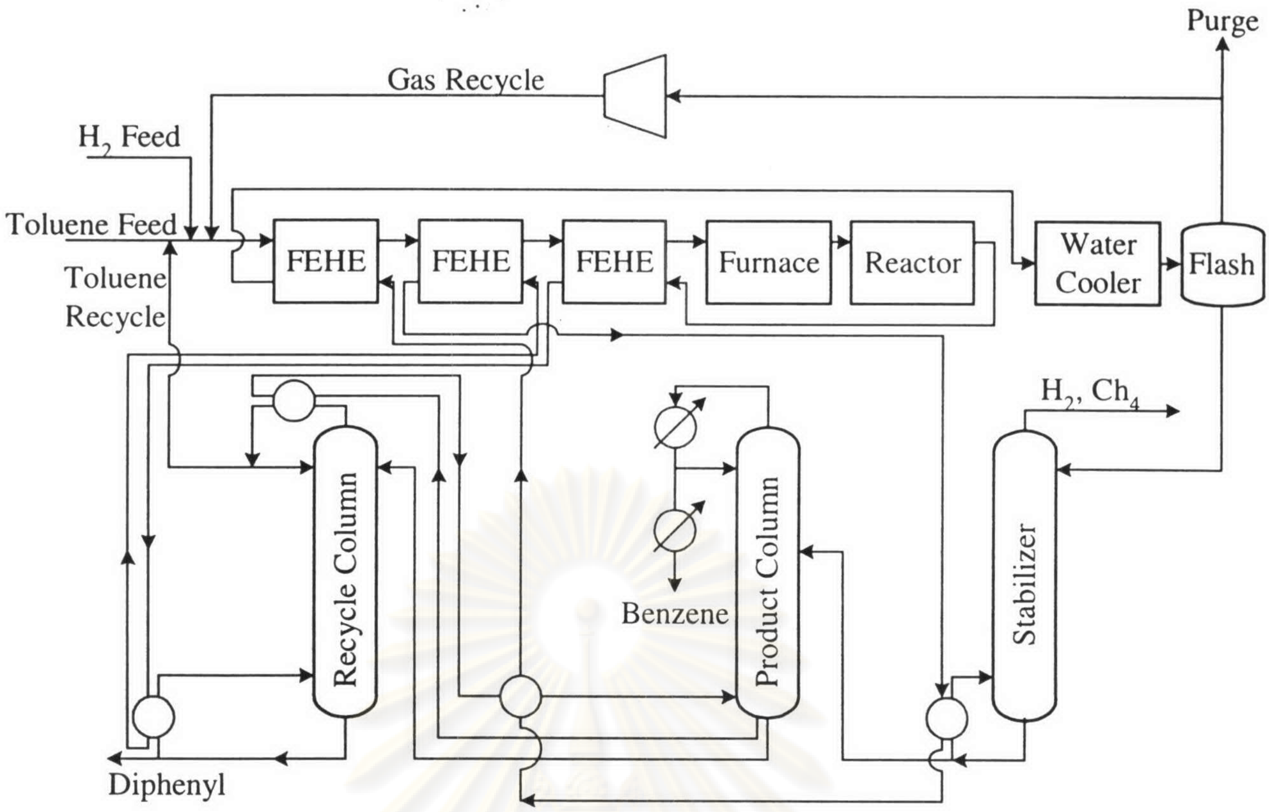


Figure 4.8 Alternative 6 For the HDA Process

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. 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 effects 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, unstable state when a sizable heat Exchanger is used. The process is simulated on DuPont's nonlinear dynamic simulator TMODS. We first verify 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 reduced. These 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 Silveratein 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.

4.6 Economics

Since cost estimates are the driving force for any design study, we need to understand the various factors to include. We describe a procedure for generating a cost estimate for a conceptual design in this chapter. We begin by resenting the results from a published case study, in order to gain an overall perspective on the types of cost data required, and then we discuss the details of the cost analysis.

Remember that the cost models that we develop should be used only for screening process alternatives. The cost estimates that are reported to management should be prepared by the appropriate economic specialists in the company, because they will include contingency factors based on experience and will include the costs of more items than we consider. Thus, our cost estimates normally will be too optimistic, and they should be kept confidential until they have been verified.

We presented a very simple economic model that we can used for conceptual designs (i.e., the screening of a large number of flowsheet alternatives by using order-of-magnitude estimates to determine the best flowsheet or the best few alternatives):

$$\text{Revenues} = \text{Raw Matl.}+\text{Util.}+\text{Ann.Install.Equip.Cost}+2.13\times10^{5}\ \text{Operators}$$

The annualized installed equipment costs are determined by multiplying the installed equipment costs by a CCF which includes all the investment-related costs.

Economic Potential

The approximate cost model presented above fits into the hierarchical framework very nicely. Thus, when we consider the input-output structure of the flowrate, i.e., level 2 in the hierarchy, we can define an economic potential EP_2 at this level as

EP_2 = Revenue-Raw Matl.- (Power+Ann.Cap.Cost of Feed Compress. If any)

Similarly, when we consider the recycle structure of the flowsheet, i.e., level 3, and we generate cost estimates for the reactor and a recycle gas compressor (if any), we can write

EP_2 = Revenue-Raw Matl. – (Feed Compress. Cap.+Op.Cost)
- Reactor Cost – (Gas-Recycle Comprocess.Cap.+Op.Cost)

Thus, as we add more detail to the flowsheet, we merely subtract the new utilities costs and the annualized, installed equipment cost of the new equipment that is added. If the economic potential at any level becomes negative, we have three options:

1. Terminate the design study.
2. Look for a better process alternative.
3. Increase the product prices so that the economic potential is zero, and continue with the design.

If we follow option 3, we eventually determine a value of the product price that would make the process alternative under consideration profitable. If this new product price were only slightly higher than the current price, we would probably continue with the design. (We need to undertake a supply-and-demand analysis to see how far in the future that we might expect to obtain this higher price.)

However, if the product price required to make the alternative profitable were much greater than the current price at any of the levels in the hierarchy, we would terminate the work on the current alternative and look for one that was cheaper. If none of the alternatives were acceptable, we would terminate the project. This approach is very efficient because it makes it possible to terminate projects with a minimum amount of design effort.