

CHAPTER II

LITERATURE REVIEW

Our purpose of this chapter is to present a review of the previous work on the conceptual design of chemical process, heat exchanger networks (HENs) and plantwide control design.

2.1 Conceptual Design

A synthesis/analysis procedure for developing first flowsheets and base case designs has been established by Douglas (1985). The procedure is described in terms of a hierarchy of decision levels, as follows:

1. Batch versus continuous
2. Input-output structure of the flowsheet
3. Recycle structure of the flowsheet
4. Separation system specification, including vapor and liquid recovery system
5. Heat exchanger network(HEN)

Douglas (1985) considered a continuous process for producing benzene by hydrodealkylation of toluene (HDA process) to illustrate the procedure. The complete process is always considered at each decision level, but additional fine structure is added to the flowsheet as he proceeds to the later decision level. Each decision level terminates in an economic analysis. Experience indicates that less than one percent of the ideals for new designs are ever commercialized, and therefore it is highly desirable to discard poor projects quickly. Similarly, the later level decisions are guided by the economic analysis of the early level decisions.

In a series of papers, Fisher et al. (1988 a, b, c) presented a study of the interface between design and control including process controllability, process operability and selecting a set of controlled variables. At the preliminary stages of a process design, most plants are uncontrollable. That is normally there are not enough manipulative variables in the flowsheet to be able to satisfy all of the process constraints and to optimize all of the operating variables as disturbances enter the plant. In order to develop a systematic procedure for controllability analysis, Fisher et al. (1988a) used the design decision hierarchy described by Douglas (1985) as the decomposition procedure and considered HDA process as a case study. Where at some levels, that are level 1, 2 and 3, the process is uncontrollable, but controllable at level 4 and level 5. If the available manipulated variables are compared with the constraints and operating variables introduced at each level, the preliminary controllability criterion can often be satisfied.

Beside controllability analysis, Fisher et al. (1988b) also focused on operability analysis. The goal of operability analysis is to ensure that there is an adequate amount of equipment over design so that they could satisfy the process constraints and minimize a combination of the operating costs and over design costs over the entire range of anticipated process disturbances. They also followed the same hierarchical procedure to develop operability analysis. For HDA process, the operability decisions were encountered at each level. Fisher et al. (1988c) proposed steady state control structure for HDA process using an optimum steady state control analysis. They found the values of manipulated variables (that minimize the total operating costs for various values of the disturbances) and used it to define the controlled variables.

D. L. Terrill and J. M. Douglas (1988) have studied HDA process from a steady state point of view and determined that the process can be held very close to its optimum for a variety of expected load disturbances by using the following strategy: (1) Fix the flow of recycle gas through the compressor at its maximum value, (2) Hold a constant heat input flowrate in the stabilizer, (3) Eliminate the reflux entirely in the recycle column, (4) Maintain a constant hydrogen-to-aromatic ratio in the reactor inlet by adjusting hydrogen fresh feed, (5) Hold the recycle toluene flowrate constant by

adjusting fuel to the furnace, (6) Hold the temperature of the cooling water leaving the partial condenser constant. Downs and Vogel (1993) described a model of an industrial chemical process for the purpose of developing, studying and evaluating process control technology. It consisted of a reactor/separator/recycle arrangement involving two simultaneous gas-liquid exothermic reactions. This process was well suited for a wide variety of studies including both plantwide control and multivariable control problems.

Tyreus and W. L. Luyben (1993) considered second order kinetics with two fresh feed makeup streams. Two cases are considered: (1) instantaneous and complete one pass conversion of one of the two components in the reactor so there is an excess of only one component that must be recycled and (2) incomplete conversion per pass so there are two recycle streams. It is shown that the generic liquid-recycle rule proposed by Luyben applies in both of these cases: "snow-balling" is prevented by fixing the flowrate somewhere in the recycle system. An additional generic rule is proposed fresh feed makeup of any component cannot be fixed unless the component undergoes complete single-pass conversion. In the complete on-pass conversion case, throughput can be set by to fix the flowrate of the limiting reactant. The makeup of the other reactant should be set by level control in the reflux drum of the distillation column.

Yi and Luyben (1995) presented a method that was aimed at helping to solve this problem by providing a preliminary screening of candidate plantwide control structures in order to eliminate some poor structures. Only steady state information was required. Equation-based algebraic equation solvers were used to find the steady state changes that occur in all manipulated variables for a candidate control structure when load changes occur. Each control structure fixed certain variables: flows, compositions, temperatures, etc. The number of fixed variables was equal to the number of degrees of freedom of the closed-loop system. If the candidate control structure required large changes in manipulated variables, the control structure was a poor one because valve saturation and equipment overloading will occur. The effectiveness of the remaining structures was demonstrated by dynamic simulation.

Some control structures were found to have multiple steady states and produce closed-loop instability.

2.2 Heat Exchanger Networks (HENs)

Linhoff, B. and Hindmarsh, E. (1983) presented a novel method for the design of HEN. The method is the first to combine sufficient simplicity to be used by hand with near certainty to identify "best" designs, even for large problems. Best design features the highest degree of energy recovery possible with a given number of capital items. Moreover, they feature network patterns required for good controllability, plant layout, intrinsic safety, etc. Typically, 20-30 percent energy savings, coupled with capital saving, can be realized in state of the art flowsheets by improved HEN design. The task involves the placement of process and utility heat exchangers to heat and cool process streams from specified supply to specified target temperatures.

Generally, minimum cost networks feature the correct degree of energy recovery and the correct number of units. This is achieved in two stages. First, the method aims for a minimum energy solution, corresponding to a specified ΔT_{min} with no more units than is compatible with minimum energy. This task is achieved through understanding of the pinch phenomenon, hence the method is called the pinch design method. Second, the method involves a controlled reduction in number of units. This may require "backing-off" from minimum utility usage.

1. The HEN problem is divided at the pinch into separate problems.
2. The design for this separate problem is started at the pinch and developed moving away from the pinch. At the pinch essential matches, match options and stream splitting requirements are identified by applying the feasibility criteria.
3. When options exist at the pinch, the engineer is free to base his selection to suit the process requirements.

4. The heat loads of exchangers at the pinch are determined using the stream tick-off heuristic. In case of difficulty, a different exchanger topology at the pinch can be chosen or the load on the offending match can be reduced.

5. Away from the pinch there is generally a free choice of matches. The procedure does not insist on particular matches but allows the designers to discriminate between matches based on his judgment and process knowledge.

Inhofe, B., Dunford, H., and Smith, R., (1983) studied heat integration of distillation columns into overall process. This study reveals that good integration between distillation and the overall process can result in column operating at effectively zero utility cost. Generally, the good integration is when the integration as column not crossing heat recovery pinches of the process and either the reboiler or the condenser being integrated with the process. If these criteria can be met, energy cost for distillation can effectively be zero.

Saboo and Morari (1983) classified flexible HENs into two classes according to the kind and magnitude of disturbances that effect the pinch location. For the temperature variation, they show that if the MER can be expressed explicitly as a function of stream supply and target conditions the problem belongs to Class I, i.e. the case that small variations in inlet temperatures do not affect the pinch temperature location. If an explicit function for the minimum utility requirement valid over the whole disturbance range does not exist, the problem is of Class II, i.e. the case that large changes in inlet temperature of flowrate variations cause the discrete changes in pinch temperature locations.

Calandranis and Stephanopoulos (1988) proposed a new approach to address the following problems: design the configuration of control loops in a network of heat exchangers and sequence the control action of the loops, to accommodate set point changes and reject load disturbances. The approach proposed exploits the structure characteristics of a HEN by identifying routes through the HEN structure that can allocate load (disturbances, or set point changes) to available sinks (external coolers or heaters). They also discussed several design issues such as the placement of bypass

lines and the restrictions imposed by the existence of a process pinch. An online, real-time planning of control actions is the essence of implementation strategies generated by an expert controller, which selects path through the HEN is to be used for each entering disturbance or set point change, and what loops should be activated (and in what sequence) to carry the associated load (disturbance or set point change) to a utility unit.

In a series papers, studies of the sensitivity of the total processing cost to heat exchanger network alternatives and steady state operability evaluation were undertaken by Terrill and Douglas (1987 a, b, c). They considered the temperature-enthalpy (T-H) diagram and developed six HEN alternatives for a base case design for HDA process which energy savings ranging between 29 and 43 percent. The simplest of these designs is alternative 1, recovers an additional 29 percent of the base case heat consumption by making the reactor preheater larger and the furnace smaller. The most complicated of the design is alternative 6, recovers 43 percent of the base case net energy consumption.

Several terms have been used in the literature to describe the additional attributes of HENs that have a capability to tolerate change in input or operational parameters while achieving the targets. Operability has been used to describe the ability of the system to perform satisfactorily under normal and abnormal conditions different design condition. Normal refers to the steady state operation while abnormal refers to the transient operation during failure, start up or shut down periods. Flexibility has been used to describe the ability of process systems to readily adjust to meet the requirement of changes, i.e. different feed stocks, product specifications or process conditions. Resiliency refers to the ability of HEN to tolerate and recover from undesirable parameter variations, and the term static resiliency or simply resiliency has been used in the same sense as flexibility. Dynamic resiliency refers to ability to handle the unsteady state operation.

Colberg (1989) suggested that flexibility should deal with planned, desirable changed that often have a discrete set of values. Whereas resilience deals with unplanned, undesirable changes which are naturally continuous values. Thus a

flexibility problem is a 'multiple period' type pf problem. A resilience problem should be a problem with a continuous range of operating conditions in the neighborhood of nominal operating points.

Wongsri, M., (1990) studied a resilient HEN design. He presented a simple but effective systematic synthesis procedure for the design of resilient HEN. His heuristic design procedure is used to design or synthesize HENs with pre-specified resiliency. It used physical and heuristic knowledge in finding resilient HEN structures. The design must not only feature minimum cost, but must also be able cope with fluctuation or changers in operating conditions. The ability of a HEN to tolerate unwanted changes is called resiliency. It should be noted that the ability of a HEN to tolerate wanted changes is called flexibility. A resilient HEN synthesis procedure was developed based on the match pattern design and a physical understanding of the disturbances propagation concept. The disturbance load propagation technique was developed from the shift approach and was used in a systematic synthesis method. The design condition was selected to be the minimum heat load condition for easy accounting and interpretation. This is a condition where all process streams are at their minimum heat loads, e.g. the input temperatures of hot streams are at the lowest and those of cold streams are at the highest.

Generating designs at a base case and some extreme conditions and combining those designs to a base design requires that the designs should be similar. However, the networks designed at extreme conditions can be very different from each other. This poses difficulties in the combination. These methods involve repetitive effort in funding a resilient structure because the resiliency objective has not been included in their models. Also, the problem of selecting extreme conditions is far from trivial. Grossmann and Morari (1984) show that the extreme conditions that seem logical can load to a poor design. Most of us would select the maximum and minimum operating conditions as design conditions. However, in their example the extreme condition is located at the intermediate value. Extra units in a combined design are then eliminated by either inspection or using optimization methods to obtain a minimum unit solution. A minimum unit solution is tested for resiliency using mathematical programming or inspection techniques.

Marselle et al. (1982) addressed the problem of synthesizing heat recovery networks, where the inlet temperatures vary within given ranges and presented the design procedure for a flexible HEN by finding the optimal network structures for four selected extreme operating conditions separately. The specified worst cases of operating conditions are the maximum heating, the maximum cooling, the maximum total exchange and the minimum total exchange. The network configurations of each worst condition are generated and combined by a designer to obtain the final design. The strategy is to derive similar design in order to have as many common units as possible in order to minimize number of units.

Linn off and Kotjabasakis (1984) developed a design procedure for operable HENs by inspection and using the concept of downstream paths, i.e. the paths that connect the disturbed variables downstream to the controlled variables. They generated HEN design alternatives by the pinch method for the nominal operating condition. Then, the alternative designs are inspected for the effects of disturbances on the controlled variables and they are removed by breaking the troublesome downstream paths. Path breaking can be done by relocating and/or removing exchangers. If this procedure is not feasible, control action is inserted into the structure.

Saboo and Morari (1984) proposed the corner point theorem which states that for temperature variation only, if a network allows MER without violating ΔT_{min} at M corner points, then the network is structurally resilient or flexible. This is the case where the constraint is convex, so examining the vertices of the polyhedron is sufficient. This procedure again can only apply to restricted classes of HEN problem. Their design procedure is similar to Marselle et al. (1982), but using two extreme cases to develop the network structure. The strategy for both procedures is finding similar optional network structures for the extreme cases and the base case design in order that they may be easily merged and not have too many units. Two extreme cases are:

1. When all streams enter at their maximum inlet temperatures and the heat capacity flowrates of hot streams are maximal and those of cold streams minimal. This is the case of maximum cooling.
2. When all streams enter at their minimum inlet temperatures and the heat capacity flowrates of hot streams are minimal and those of cold streams maximal. This is an opposite case the above one and in this case maximum heating is required.

The 'base' design is then generated by using an optimization technique and the final design is obtained by combining these designs. A test for resiliency (calculating, RI) is required. If the design is not feasible a modification is done by attempting to reduce ΔT_{min} and if not successful, a new heat exchanger will added or some heat exchangers are located. If the modified network is still not resilient, synthesize network structures at all corner points where the current design is not feasible. The new structures should be as similar to the current design as possible. The new design is obtained by superimposing the current structure and the new structures. The unneeded heat exchangers are inspected and removed.

Floudas and Grossmann (1987) presented a synthesis procedure for resilient HENs. Their multiperiod operation transshipment model is used to find a match structure for selected design points. The design obtained for feasibility at the match level. If it is not feasible, the critical point is added as an additional operating point and the problem is reformulated and solved. If the match network is feasible then the multiperiod superstructure is derived and formulated as an NLP problem to find a minimum unit solution.

Ploypaisangsang A., (2003) presented to redesign six alternatives for HAD process to be the resiliency networks for maintain the target temperature and also achieve maximum energy recovery (MER). The best resilient network is selected by to trade-off between cost and resiliency. The auxiliary unit should be added in the network for cope safely with the variations and easy to design control structure to the network.

2.3 Design and Control of Heat-Integrated Process

In the last few decades, Douglas, Orcutt, and Berthiaume (1962) studied design and control of feed-effluent heat exchanger - reactor systems. They obtained a simultaneous solution of the steady state heat and material balances for a first order reaction occurring in the system and used it to calculate the values of exchanger and reactor lengths that minimized the equipment cost of the system. A dynamic study indicated that the desired steady state conditions were metastable. However, proportional controller could be used to stabilize the process.

Silverstein and Shinnar (1982) discussed the linear and nonlinear stability analysis of a fixed bed catalytic reactor with heat exchanger between the feed and product streams, with special emphasis on case which are open loop unstable. They used classical frequency response techniques, contains the implicit assumption that the designer should evaluate the effect of the overall design on stability. Tyreus, B.D. and Luyben, W. L., (1993) presented a mathematical analysis of the unusual dynamic in coupled reactor/preheater process. The outlet temperature of the reactor exhibits inverse response for a change in the inlet reactor temperature and a large dead time.

Handogo, R. and Luyben, W. L., (1987) studied the dynamics and control of a heat-integrated reactor/column system. An exothermic reactor was the heat source, and a distillation column reboiler was the heat sink. Two types of heat-integrated system were examined: indirect and direct heat integration. Both indirect and direct heat-integration systems are found in industry. In the indirect heat-integration system, steam generation was used to cool the reactor, and the steam was used as the heating medium for the reboiler. The direct heat-integration system used the reactor fluid to directly heat the column reboiler. The indirect heat-integration system was found to have several advantages over the direct heat-integration system in terms of its dynamic performance. Both systems were operable for both large and small temperature differences between the reactor and column base. Somewhat unexpectedly, the heat-integration system with a small temperature difference was found to be more controllable than a system with a larger temperature difference.

However, the cost of the heat exchanger increased rapidly as the temperature difference decreased. An important thing in this study is how to solve some of control difficulties in the process associated with heat integration schemes. They suggested adding auxiliary utility coolers and reboilers to the process.

M.L. Luyben and W.L. Luyben (1995) examined the plantwide design and control of a complex process. The plant contains two reactions steps, three distillation columns, two recycle streams, and six chemical components. Two methods, a heuristic design procedure and a nonlinear optimization, have been used to determine an approximate economically optimal steady state design. The designs differ substantially in terms of the purities and flowrates of the recycle streams. The total annual cost of the nonlinear optimization design is about 20 percent less than the cost of the heuristic design. An analysis has also been done to examine the sensitivity to design parameters and specifications. Two effect control strategies have been developed using guidelines from previous plantwide control studies; both require reactor composition control as well as flow control of a stream somewhere in each recycle loop. Several alternative control strategies that might initially have seemed obvious do not work.

Jones, W.E., and Wilson, J.A., (1997) considered the range ability of flows in the bypass line of heat exchanger through interesting heat exchanger problems. Difficulty is immediately encountered when considering heat exchanger between two process streams; changing the flowrate of one will certainly affect the exit temperature of the other. Unfortunately, interfering with a process stream flowrate immediately upsets the plant mass balance, which is undesirable. The difficulty is overcome by using a bypass that does not affect the total flowrate but changes the proportion actually passing through the heat exchanger and hence the heat transfer. Good engineering practice would maintain a minimum flowrate of 5-10 percent through the bypass. This bypass is expected to be able to handle disturbances.

Luyben, M.L., Tyreus, B.D. and Luyben, W.L., (1997) presented a general heuristic design procedure. Their procedure generated an effective plantwide control structure for an entire complex process flowsheet and not simply individual units. The

nine step of the proposed procedure center around the fundamental principles of plantwide control: energy management, production rate, product quality, operational, environmental and safety constraints, liquid-level and gas-pressure inventories, makeup of reactants, component balances and economic or process optimization. Application of the procedure was illustrated with three industrial examples: the vinyl acetate monomer process, Eastman process and HDA process. The procedure produced a workable plantwide control strategy for a given process design. The control system was tested on a dynamic model built with TMODS, DuPont's in-house simulator.

From the W.L. Luyben (2000) studied the process had the exothermic, irreversible, gas - phase reaction $A + B \rightarrow C$ occurring in an adiabatic tubular reactor. A gas recycle returns unconverted reactants from the separation section. Four alternative plantwide control structures for achieving reactor exit temperature control were explored. The reactor exit temperature controller changed different manipulated variables in three of the four control schemes: (1) CS1, the setpoint of the reactor inlet temperature controller was changed; (2) CS2, the recycle flowrate was changed; and (3) CS3, the flowrate of one of the reactant fresh feeds was changed. The fourth control scheme, CS4, uses an "on - demand" structure. Looking that the dynamics of the reactor in isolation would lead one to select CS2 because CS1 had a very large deadtime and CS3 had a very small gain. Dynamic simulations demonstrated that in the plantwide environment, with the reactor and separation operating together, the CS3 structure gave effective control and offered an attractive alternative in those cases where manipulation of recycle flowrate was undesirable because of compressor limitations. The on - demand CS4 structure was the best for handling feed composition disturbances. Kunlawaniteewat, J.,(2001) proposed the rules and procedure for design control structure of heat exchanger network using heuristic approach for to achieve outlet temperature targets and maintain maximum energy recovery (MER). The rules are categorized as following: generals, match pattern, loop placement, bypass placement, and split fraction rules.

Wongsri and Kietawarin (2002) presented a comparison among four control structures designed for withstanding disturbances that cause production rate change of

HDA process. The changes had been introduced to the amount of toluene and feed temperature before entering the reactor. Compared with the reference control structure using a level control to control toluene quantity in the system, the first control scheme measured toluene flowrate in the process and adjusted the fresh toluene feed rate. This structure resulted in faster dynamic response than the reference structure. The second control scheme was modified from the first scheme by adding a cooling unit to control the outlet temperature from the reactor, instead of using internal process flow. The result was to reduce material and separation ratio fluctuations within the process. The product quality was also quite steadily. In the third control scheme, a ratio control was introduced to the second control scheme for controlling the ratio of hydrogen and toluene within the process. This scheme showed that it could withstand large disturbances. Dynamic study showed that the control structure had significant effect on process behavior. A good system control should quickly response to disturbances and adjusts itself to steady state while minimizing the deviation of the product quality.

Chen, T.H., and Yu, C.C. (2003) proposed systematic approach to complex FEHE schemes. Because a loss of controllability come the positive feedback loop, several design parameters were studied, and the design heuristic were proposed to give more controllable heat integration schemes. They used two examples, a simple two-FEHE example and an HDA process example to illustrate the assessment of controllability based on process flowsheet. The results showed that, contrary to expectations, some complex heat-integrated reactor design alternatives (e.g., alternative 6 of HDA example) were indeed more controllable than some of the simpler heat-integration schemes (e.g., alternative 1). The increased number of FEHEs allows for a greater number of candidate manipulated inputs and thus provides opportunities for multivariable control.

Wongsri and Thaicharoen (2004) presented the new control structures for HDA process with energy integration schemes alternative 3. Five control structures have been designed, tested and compared the performance with Luyben's structure (CS1). The result showed that the HDA process with heat integration can reduce energy cost. Furthermore, this process can be operated well by using plantwide methodology to design the control structure. The dynamics responses of the designed

control structures and the reference structure are similar. The CS2 has been limited in bypass. So, it is able to handle in small disturbances. The CS3 has been designed to improve CS2 in order to handle more disturbances by using auxiliary heater instead of bypass valve to control temperature of stabilizer column. The recycle column temperature control response of the CS4 is faster than that of the previous control structures, because reboiler duty of column can control the column temperature more effective than bottom flow. The CS5, on-demand structure has an advantage when downstream customer desires immediate responses in the availability of the product stream from this process. The energy used in CS6 control structure is less than CS1 and CS4.

Wongsri and Hermawan Y.D., (2004) studied the control strategies for energy integrated HDA plant (i.e. alternative 1, 4 and 6) based on the heat pathway heuristics, i.e. selecting an appropriate heat pathway to carry associated load to a utility unit, so that the dynamic maximum energy recovery (DMER) can be achieved with some trade-off. In addition, a selective controller with low selector switch (LSS) is employed to select an appropriate heat pathway through the network. The new control structure with the LSS has been applied in the HDA plant.