Chapter

1

The Hierarchy of Chemical Process Design

1.1 Introduction

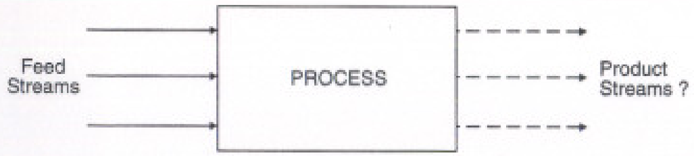
In a chemical process, the transformation of raw materials into desired products usually cannot be achieved in a single step. Instead, the overall transformation is broken down into a number of steps that provide intermediate transformations. These are carried out through reaction, separation, mixing, heating, cooling, pressure change, particle size reduction and enlargement, etc. Once individual steps have been selected, they must be interconnected to carry out the overall transformation (Fig. 1.1*a*). Thus the *synthesis* of a chemical process involves two broad activities. First, individual transformation steps are selected. Second, these individual transformations are interconnected to form a complete structure that achieves the required overall transformation. A *flowsheet* is the diagrammatic representation of the process steps with their interconnections.

Once the flowsheet structure has been defined, a *simulation* of the process can be carried out. A simulation is a mathematical model of the process which attempts to predict how the process would behave if it was constructed (see Fig. 1.1*b*). Having created a model of the process, we assume the flow rates, compositions, temperatures, and pressures of the feeds. The simulation model then predicts the flow rates, compositions, temperatures, and pressures of the products. It also allows the individual items of equipment in the process to be sized and predicts how much raw material is being used, how much energy is being consumed, etc. The performance of the design can then be evaluated.

There are many facets to the evaluation of performance. Good economic performance is an obvious first criterion, but it is certainly not the only one. Chemical processes should be designed as part of a sustainable industrial development which retains the capacity of ecosystems to support both industrial activity and life. In practical terms this means that waste should be minimized and that any waste byproducts which are produced must not be environmentally harmful. Sustainable development also demands that the process should use as little energy as practicable. The process also must meet required health and safety criteria. Start-up, emergency shutdown, and ease of control are other important factors. Flexibility, i.e., the ability to operate under different conditions such as differences in feedstock and product specification, etc., may be important. Availability, i.e., the number of operating hours per year, also may be important. Some of these factors, such as economic performance, can be readily quantified; others, such as safety, often cannot. Evaluation of the factors which are not readily quantifiable, the intangibles, requires the judgment of the designer.

Once the basic performance of the design has been evaluated, changes can be made to improve the performance; in other words, we *optimize*. These changes might involve the synthesis of alternative structures, i.e., *structural optimization*. Thus we simulate and evaluate again, and so on, optimizing the structure. Alternatively, each structure can be subjected to *parameter optimization* by changing operating conditions within that structure.

(a) Process design starts with the synthesis of a process to convert raw materials into desired products.



(b) Simulation predicts how a process would behave if it was constructed.

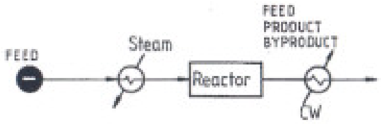
Figure 1.1 Synthesis is the creation of a process to transform feed streams into product streams. Simulation predicts how it would behave if it was constructed.

We might think that we can find all the structural options by inspection, at least all of the significant ones. The fact that even long-established processes are still being improved bears evidence to just how difficult this is.

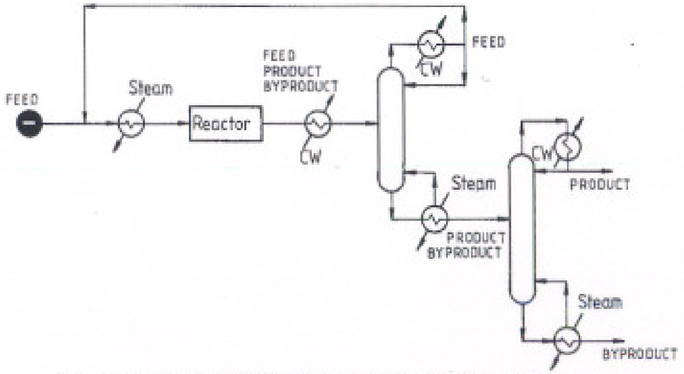
This text will attempt to develop an understanding of the concepts required at each stage during the creation of a chemical process design.

1.2 Overall Process Design

Consider the process illustrated in Fig. 1.2.[1] The process requires a reactor to transform the FEED into PRODUCT (Fig. 1.2*a*). Unfortunately, not all the FEED reacts. Also, part of the FEED reacts to form BYPRODUCT instead of the desired PRODUCT. A



(a) A reactor transforms FEED into PRODUCT and BYPRODUCT.



(b) To isolate the PRODUCT and recycle unreacted FEED we need a separation system.

Figure 1.2 Process design starts with the reactor. The reactor design dictates the separation and recycle problem. *(From Smith and Linnhoff, Trans. IChemE, ChERD, 66:195, 1988; reproduced by permission of the Institution of Chemical Engineers.)*

separation system is needed to isolate the PRODUCT at the required purity. Figure 1.2*b* shows one possible separation system consisting of two distillation columns. The unreacted FEED in Fig. 1.2*b* is recycled, and the PRODUCT and BYPRODUCT are removed from the process. Figure 1.2*b* shows a flowsheet in which all heating and cooling is provided by external utilities (steam and cooling water in this case). This flowsheet is probably too inefficient in its use of energy, and we would attempt to recover heat. Thus we *heat integrate* and exchange heat between those streams which need to be cooled and those which need to be heated. Figure 1.3 shows two possible designs for the *heat exchanger network*, but many other heat integration arrangements are possible.

The flowsheets shown in Fig. 1.3 feature the same reactor design. It could be useful to explore changes in reactor design.[1] For example, the size of the reactor could be increased to increase the amount of FEED which reacts (Fig. 1.4*a*). Now there is not only much less FEED in the reactor effluent but more PRODUCT and BYPRODUCT. However, the increase in BYPRODUCT is larger than the increase in PRODUCT. Thus, although the reactor in Fig. 1.4*a* has the same three components in its effluent as the reactor in Fig. 1.2*a*, there is less FEED, more PRODUCT, and significantly more BYPRODUCT. This change in reactor design generates a different task for the separation system, and it is possible that a separation system different from that shown in Figs. 1.2 and 1.3 is now appropriate. Figure 1.4*b* shows a possible alternative. This also uses two distillation columns, but the separations are carried out in a different order.

Figure 1.4*b* shows a flowsheet without any heat integration for the different reactor and separation system. As before, this is probably too inefficient in the use of energy, and heat integration schemes can be explored. Figure 1.5 shows two of the many possible flowsheets.

Different complete flowsheets can be evaluated by simulation and costing. On this basis, the flowsheet in Fig. 1.3*b* might be more promising than the flowsheets in Figs. 1.3*a*, 1.5*a*, and 1.5*b*. However, we cannot be sure that we have the best flowsheet without first optimizing the operating conditions for each. The flowsheet in Fig. 1.5*b* might have greater scope for improvement than that in Fig. 1.3*b*.

Thus the complexity of chemical process synthesis is twofold.[1] First, can we identify all possible structures? Second, can we optimize each structure for a valid comparison? When optimizing the structure, there may be many ways in which each individual task can be performed and many ways in which the individual tasks can be interconnected. This means that we must simulate and optimize operating conditions for a multitude of structural options. At first sight this appears to be an overwhelmingly complex problem.

1.3 The Hierarchy of Process Design and the Onion Model

Our attempt to develop a methodology will be helped if we have a clearer picture of the structure of the problem. If the process requires a reactor, this is where the design starts. This is likely to be the only

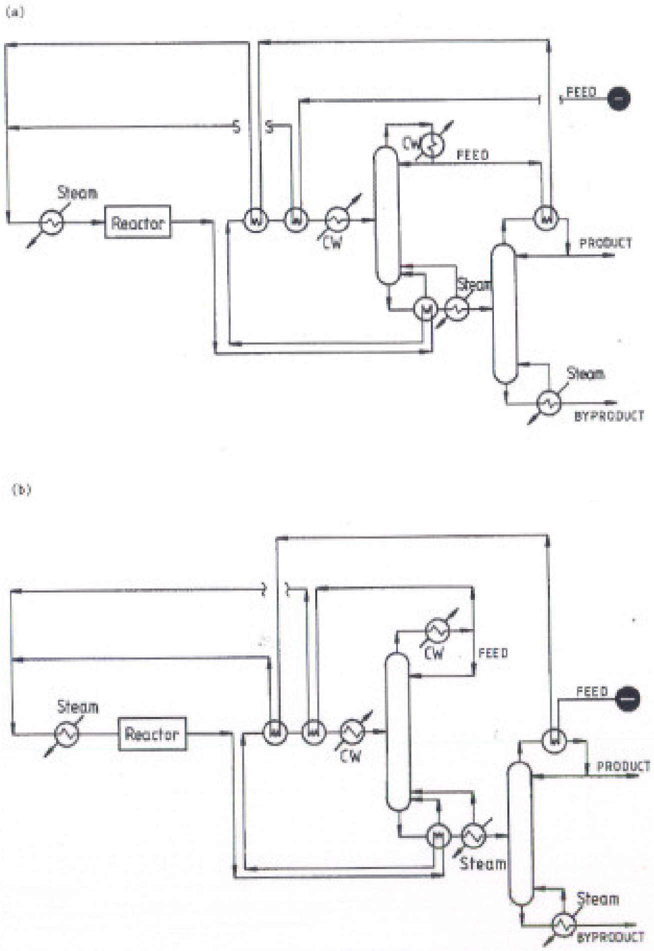
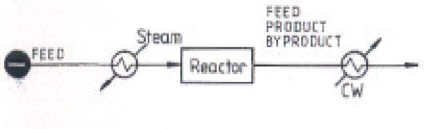


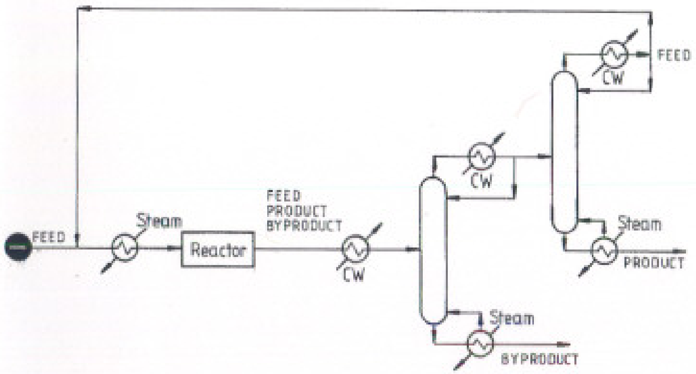
Figure 1.3 For a given reactor and separator design, there are different possibilities for heat integration. *(From Smith and Linnhoff, Trans. IChemE, ChERD, 66:195, 1988; reproduced by permission of the Institution of Chemical Engineers.)*

place in the process where raw materials are converted into products. The chosen reactor design produces a mixture of unreacted feed materials, products, and byproducts that need separating. Unreacted feed material is recycled. The reactor design dictates the separation and recycle problem. Thus design of the separation and recycle system follows reactor design. The reactor and separation and recycle system designs together define the process heating and cooling duties. Thus heat exchanger network design comes third. Those heating and cooling duties which cannot be satisfied by heat recovery dictate the need for external *utilities* (steam, cooling water, etc.). Thus utility selection and design come fourth. This hierarchy can be represented symbolically by the layers of the "onion diagram" shown in Fig. 1.6.[2] The diagram emphasizes the sequential, or hierarchical, nature of process design.

Of course, some processes do not require a reactor, e.g., some oil refinery processes. Here, the design starts with the separation system and moves outward to the heat exchanger network and utilities. However, the basic hierarchy prevails.



(a) Changing the reactor design decreases the unreacted FEED, increases the PRODUCT, and significantly increases the BYPRODUCT.



(b) The alternative reactor design calls for a different separation system.

Figure 1.4 Changing the reactor dictates a different separation and recycle problem. *(From Smith and Linnhoff, Trans. IChemE, ChERD, 66:195, 1988, reproduced by permission of the Institution of Chemical Engineers.)*

The hierarchical nature of process design has been represented in different ways by different authors. A *hierarchy of decisions*[3] and a *process design ladder*[4] also have been suggested.

The synthesis of the correct structure and the optimization of parameters in the design of the reaction and separation systems are often the single most important tasks of process design. Usually there are many options, and it is impossible to fully evaluate them unless a complete design is furnished for the "outer layers" of the onion. For example, it is not possible to assess which is better,

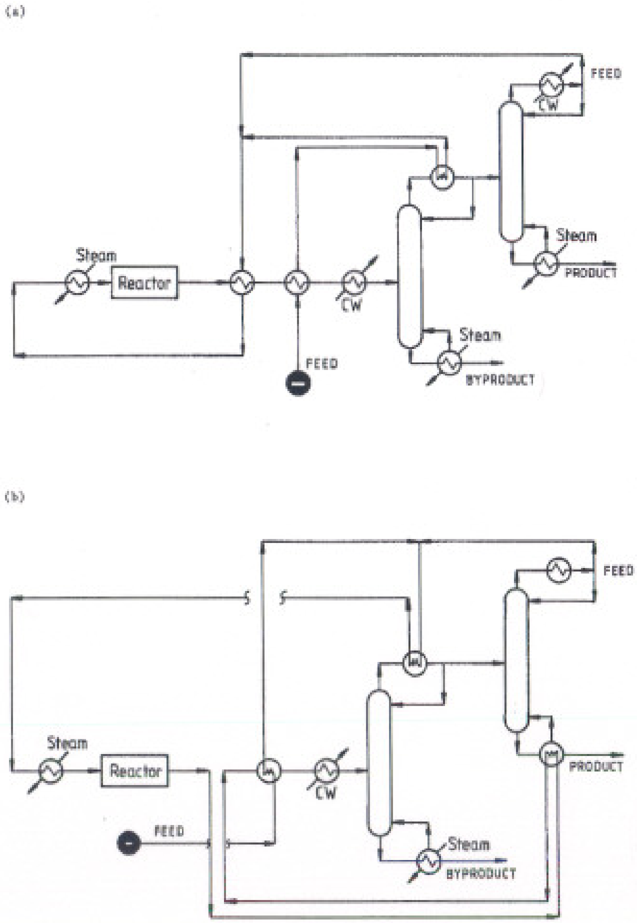


Figure 1.5 A different reactor design leads not only to a different separation system but also to additional possibilities for heat integration. *(From Smith and Linnhoff, Trans. IChemE, ChERD, 66:195, 1988; reproduced by permission of the Institution of Chemical Engineers.)*

the basic scheme from Fig. 1.2*b* or that from Fig. 1.4*b*, without fully evaluating all possible designs such as shown in Figs. 1.3*a* and *b* and 1.5*a* and *b*, etc., all completed, including utilities, etc. Such a complete search is normally too time consuming to be practical.

Later in this text an approach is presented in which some early decisions (i.e., decisions regarding reactor and separator options) can be evaluated without a complete design for the outer layers.[1]

1.4 Approaches to Process Design

In broad terms, there are two approaches to chemical process design:

1. *Building an irreducible structure.* The first approach follows the "onion logic," starting the design by choosing a reactor and then moving outward by adding a separation and recycle system, and so on. At each layer we must make decisions based on the information available at that stage. The ability to look ahead to the completed design might lead to different decisions. Unfortunately, this is not possible, and instead, decisions must be based on an incomplete picture.

This approach to synthesis is one of making a series of best local decisions. Equipment is added only if it can be justified economically on the basis of the information available, albeit an incomplete picture. This keeps the structure irreducible, and features which are technically or economically redundant are not included.

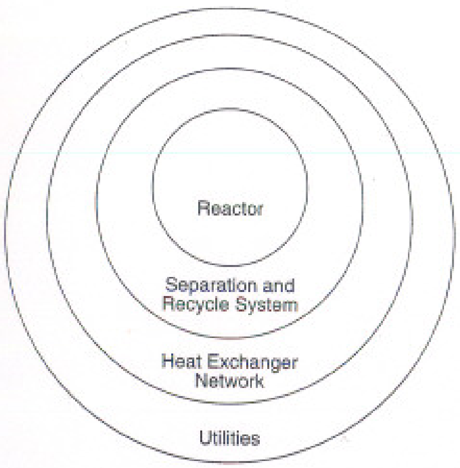


Figure 1.6 The "onion model" of process design. A reactor design is needed before the separation and recycle system can be designed, and so on. *(From Smith and Linnhoff, Trans. IChemE, ChERD, 66:195, 1988; reproduced by permission of the Institution of Chemical Engineers.)*

There are two drawbacks to this approach:

a. Different decisions are possible at each stage of the design. To be sure we have made the best decisions, the other options must be evaluated. However, each option cannot be evaluated properly without completing the design for that option and optimizing the operating conditions. This means that many designs must be completed and optimized in order to find the best.
b. Even completing and evaluating many options gives no guarantee of ultimately finding the best possible design. Complex interactions can occur between different items of equipment in a flowsheet. The effort to keep the system simple and to not add equipment in the early stages of design may result in missing the benefit of interactions between different items of equipment in a more complex system.

The main advantage of this approach is that the designer can keep control of the basic decisions and interact with the design as it develops. By staying in control of the basic decisions, the intangibles of the design can be included in the decision making.

2. *Creating and optimizing a reducible structure.* In this approach, a structure known as a *superstructure* or *hyperstructure* is first created that has embedded within it all feasible process operations and all feasible interconnections that are candidates for an optimal design.[5] Initially, redundant features are built into the structure. As an example, consider Fig. 1.7. This shows one possible structure of a process for the manufacture of benzene from the reaction between toluene and hydrogen.[6] In Fig. 1.7, the hydrogen enters the process with a small amount of methane as an impurity. Thus in Fig. 1.7 the option is embedded of either purifying the hydrogen feed with a membrane or passing directly to the process. The hydrogen and toluene are mixed and preheated to reaction temperature. Only a furnace has been considered feasible in this case because of the high temperature required. Then two alternative reactor options, isothermal and adiabatic reactors, are embedded, and so on. Redundant features have been included in an effort to ensure that all features that could be part of an optimal solution have been included.

The design problem is next formulated as a mathematical problem with *design equations* and *design variables*. The design equations are the modeling equations of the units and their specification constraints. Design variables are of two types. The first type of design variables describe the operation of each unit (flow rate, composition, temperature, and pressure), its size (volume, heat transfer area, etc.), as well as the costs or profits associated with the units. Since

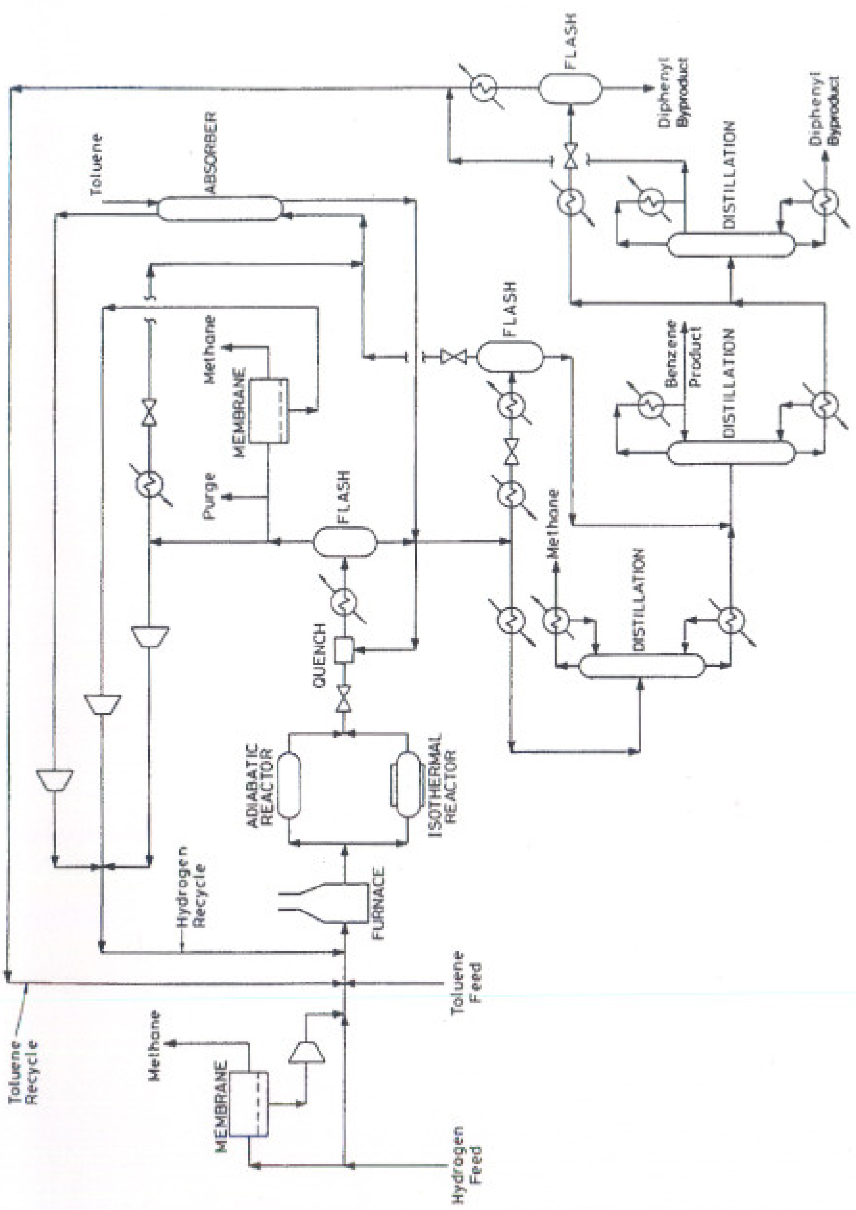


Figure 1.7 An initial structure for the manufacture of benzene from toluene and hydrogen incorporating some redundant features.

the dependence of the design equations on these variables is described in a continuous manner, they are known as *continuous variables*. The second type of design variables, known as *integer variables*, concern decisions on the structure of the flowsheet. These describe the existence of a particular unit or connection. They take on a value of unity if the unit or connection exists and a value of zero otherwise.

Once the problem is formulated mathematically, its solution is carried out through implementation of an optimization algorithm. Economic potential is maximized or cost is minimized (see App. A) in a *structural and parameter optimization*. Should an integer variable be optimized to zero, the corresponding feature is deleted from the structure and the structure is reduced in complexity. In effect, the discrete decision-making aspects of process design are replaced by a discrete/continuous optimization. Thus the initial structure in Fig. 1.7 is optimized to reduce the structure to the final design shown in Fig. 1.8. In Fig. 1.8, the membrane separator on the hydrogen feed has been removed by optimization, as have the isothermal reactor and many other features of the initial structure shown in Fig. 1.7.

There are a number of difficulties associated with this approach:

a. The approach will fail to find the optimal structure if the initial structure does not have the optimal structure embedded somewhere within it. The more options included, the more likely it will be that the optimal structure has been included.

b. If the individual unit operations are represented accurately, the resulting economic potential profile (see App. A) that must be optimized is both extremely large and irregular. The economic-potential profile is rather like the terrain in a range of mountains with many peaks. Each peak in the mountain range represents a *local optimum* in the economic potential. The highest peak represents the point of maximum economic potential and is the *global optimum*. Optimization requires searching around the mountains in a thick fog to find the highest peak, without the benefit of a map and only a compass to tell direction and an altimeter to show height. On reaching the top of any peak, there is no way of knowing whether it is the highest peak because of the fog. All peaks must be searched to find the highest. There are crevasses into which we might fall and not be able to climb out. Such problems can be overcome by changing the model such that the solution space becomes more regular, making the optimization simpler. This most often means simplifying the representation of the operations to make the representation as linear as possible.

c. The most serious drawback is that the design engineer is removed from the decision making. Thus the many intangibles in design,

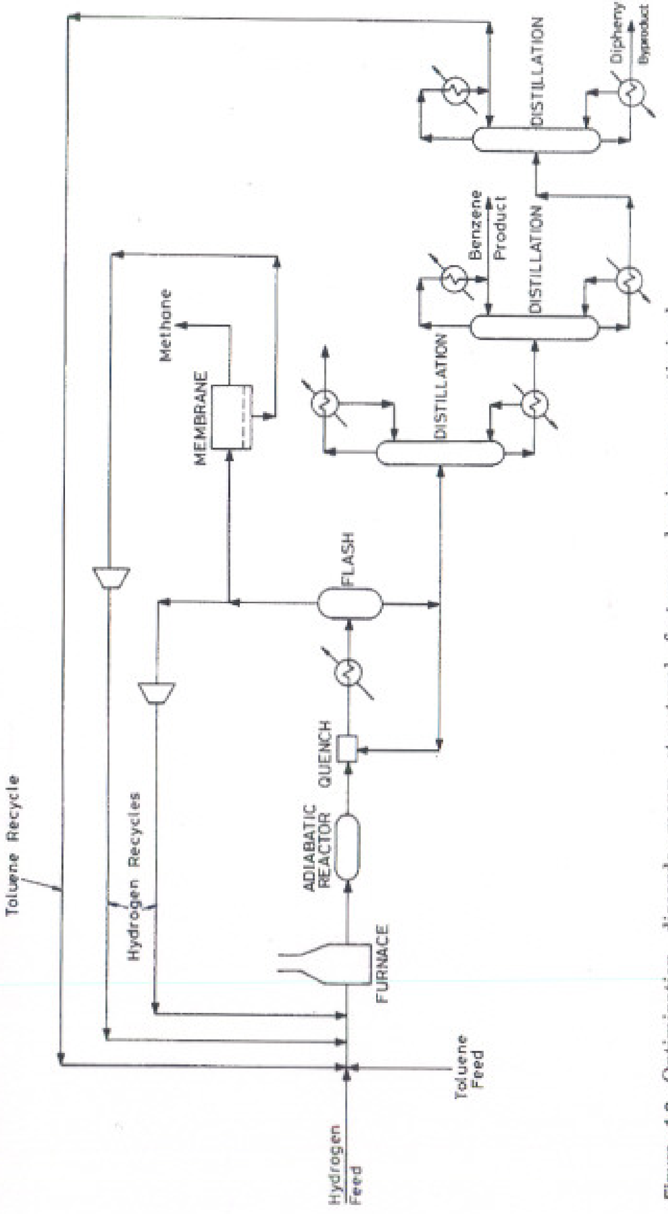


Figure 1.8 Optimization discards many structural features, leaving an optimized structure.

such as safety, layout, etc., which are difficult to include in the mathematical formulation, cannot be taken into account satisfactorily.

On the other hand, this approach has a number of advantages. Many different design options can be considered at the same time. Also, the entire design procedure can be accommodated in a computer program capable of producing designs quickly and efficiently.

In summary, the two general approaches to chemical process design of building an irreducible structure and creating and optimizing a reducible structure both have advantages and disadvantages. Whichever is used in practice, however, there is no substitute for understanding the problem.

This text concentrates on developing an understanding of the concepts required at each stage of the chemical process design. Such understanding is a vital part of process design, whichever approach is followed.

1.5 The Hierarchy of Chemical Process Design—Summary

When developing a chemical process design, there are two basic problems:

- Can all possible structures be identified?
- Can each structure be optimized such that all structures can be compared on a valid basis?

Design starts at the reactor because it is likely to be the only place in the process where raw materials are converted into desired products. The reactor design dictates the separation and recycle problem. The reactor design and separation and recycle problem together dictate the heating and cooling duties for the heat exchanger network. Those duties which cannot be satisfied by heat recovery dictate the need for external utilities. This hierarchy is represented by the layers in the "onion diagram" (see Fig. 1.6).

There are two general approaches to chemical process design:

- Building an irreducible structure
- Creating and optimizing a reducible structure

Both these approaches have advantages and disadvantages.

1.6 References

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