Chapter 1

The Nature of Chemical Process Design and Integration

1.1 Chemical Products

Chemical products are essential to modern living standards. Almost all aspects of everyday life are supported by chemical products in one way or another. However, society tends to take these products for granted, even though a high quality of life fundamentally depends on them.

When considering the design of processes for the manufacture of chemical products, the market into which they are being sold fundamentally influences the objectives and priorities in the design. Chemical products can be divided into three broad classes:

1) *Commodity or bulk chemicals.* These are produced in large volumes and purchased on the basis of chemical composition, purity and price. Examples are sulfuric acid, nitrogen, oxygen, ethylene and chlorine.
2) *Fine chemicals.* These are produced in small volumes and purchased on the basis of chemical composition, purity and price. Examples are chloropropylene oxide (used for the manufacture of epoxy resins, ion-exchange resins and other products), dimethyl formamide (used, for example, as a solvent, reaction medium and intermediate in the manufacture of pharmaceuticals), *n*-butyric acid (used in beverages, flavorings, fragrances and other products) and barium titanate powder (used for the manufacture of electronic capacitors).
3) *Specialty or effect or functional chemicals.* These are purchased because of their effect (or function), rather than their chemical composition. Examples are pharmaceuticals, pesticides, dyestuffs, perfumes and flavorings.

Because commodity and fine chemicals tend to be purchased on the basis of their chemical composition alone, they can be considered to be *undifferentiated*. For example, there is nothing to choose between 99.9% benzene made by one manufacturer and that made by another manufacturer, other than price and delivery issues. On the other hand, specialty chemicals tend to be purchased on the basis of their effect or function and therefore can be considered to be *differentiated*. For example, competitive pharmaceutical products are differentiated according to the efficacy of the product, rather than chemical composition. An adhesive is purchased on the basis of its ability to stick things together, rather than its chemical composition, and so on.

However, in practice few products are completely undifferentiated and few completely differentiated. Commodity and fine chemical products might have impurity specifications as well as purity specifications. Traces of impurities can, in some cases, give some differentiation between different manufacturers of commodity and fine chemicals. For example, 99.9% acrylic acid might be considered to be an undifferentiated product. However, traces of impurities, at concentrations of a few parts per million, can interfere with some of the reactions in which it is used and can have important implications for some of its uses. Such impurities might differ between different manufacturing processes. Not all specialty products are differentiated. For example, pharmaceutical products like aspirin (acetylsalicylic acid) are undifferentiated. Different manufacturers can produce aspirin, and there is nothing to choose between these products, other than the price and differentiation created through marketing of the product. Thus, the terms undifferentiated and differentiated are more relative than absolute terms.

The scale of production also differs between the three classes of chemical products. Fine and specialty chemicals tend to be produced in volumes less than $1000\,t{\cdot}y^{-1}$. By contrast, commodity chemicals tend to be produced in much larger volumes than this. However, the distinction is again not so clear. Polymers are differentiated products because they are purchased on the basis of their mechanical properties, but can be produced in quantities significantly higher than $1000\,t{\cdot}y^{-1}$.

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When a new chemical product is first developed, it can often be protected by a patent in the early years of its commercial exploitation. For a product to be eligible to be patented, it must be novel, useful and unobvious. If patent protection can be obtained, this effectively gives the producer a monopoly for commercial exploitation of the product until the patent expires. Patent protection lasts for 20 years from the filing date of the patent. Once the patent expires, competitors can join in and manufacture the product. If competitors cannot wait until the patent expires, then alternative competing products must be developed.

Another way to protect a competitive edge for a new product is to protect it by secrecy. The formula for Coca-Cola has been kept a secret for over 100 years. Potentially, there is no time limit on such protection. However, for the protection through secrecy to be viable, competitors must not be able to reproduce the product from chemical analysis. This is likely to be the case only for certain classes of specialty chemicals and food products for which the properties of the product depend on both the chemical composition and the method of manufacture.

Figure 1.1 illustrates different product *life cycles* (Sharratt, 1997; Brennan, 1998). The general trend is that when a new product is introduced into the market, the sales grow slowly until the market is established and then more rapidly once the market is established. If there is patent protection, then competitors will not be able to exploit the same product commercially until the patent expires, when competitors can produce the same product and take market share. It is expected that competitive products will cause sales to diminish later in the product life cycle until sales become so low that a company would be expected to withdraw from the market. In Figure 1.1, Product *A* appears to be a poor product that has a short life with low sales volume. It might be that it cannot compete well with other competitive products and alternative products quickly force the company out of that business. However, a low sales volume is not the main criterion to withdraw a product from the market. It might be that a product with low volume finds a market niche and can be sold for a high value. On the other hand, if it were competing with other products with similar functions in the same market sector, which keeps both the sale price and volume low, then it would seem wise to withdraw from the market. Product *B* in Figure 1.1 appears to be a better product, showing a longer life cycle and higher sales volume. This has patent protection but sales decrease rapidly after patent protection is lost, leading to loss of market through competition. Product *C* in Figure 1.1 is an even better product. This shows high sales volume with the life of the product extended through reformulation of the product (Sharratt, 1997). Finally, Product *D* in Figure 1.1 shows a product life cycle that is typical of commodity chemicals. Commodity chemicals tend not to exhibit the same kind of life cycles as fine and specialty chemicals. In the early years of the commercial exploitation, the sales volume grows rapidly to a high volume, but then volume does not decline and enters a mature period of slow growth, or, in some exceptional cases, slow decline. This is because commodity chemicals tend to have a diverse range of uses. Even though competition might take away some end uses, new end uses are introduced, leading to an extended life cycle.

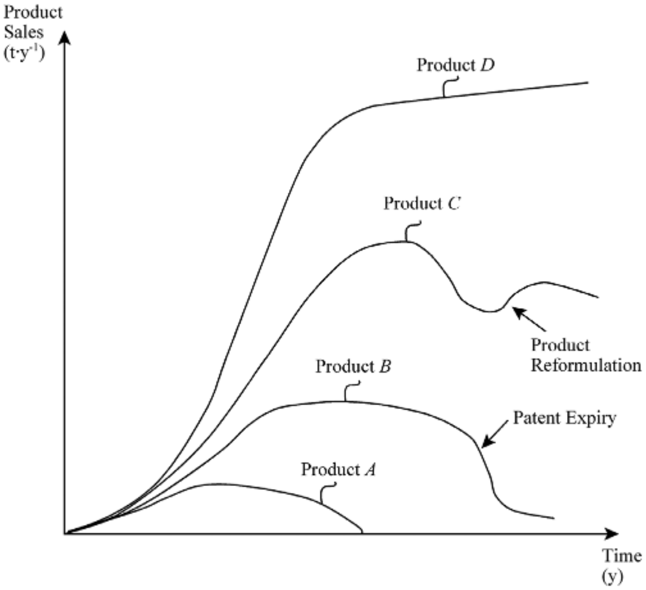


Figure 1.1

Product life cycles. (Adapted from Sharratt PN, 1997, Handbook of Batch Process Design, Chapman & Hall, reproduced by permission.)

The different classes of chemical products will have very different *added value* (the difference between the selling price of the product and the purchase cost of raw materials). Commodity chemicals tend to have low added value, whereas fine and specialty chemicals tend to have high added value. Commodity chemicals tend to be produced in large volumes with low added value, while fine and specialty chemicals tend to be produced in small volumes with high added value.

Because of this, when designing a process for a commodity chemical, it is usually important to keep operating costs as low as possible. The capital cost of the process will tend to be high relative to a process for fine or specialty chemicals because of the scale of production.

When designing a process for specialty chemicals, priority tends to be given to the product, rather than to the process. This is because the unique function of the product must be protected. The process is likely to be small scale and operating costs tend to be less important than with commodity chemical processes. The capital cost of the process will be low relative to commodity chemical processes because of the scale. The time to market for the product is also likely to be important with specialty chemicals, especially if there is patent protection. If this is the case, then anything that shortens the time from basic research, through product testing, pilot plant studies, process design, construction of the plant to product manufacture will have an important influence on the overall project profitability.

All this means that the priorities in process design are likely to differ significantly, depending on whether a process is being designed for the manufacture of a commodity, fine or specialty chemical. In commodity chemicals, there is likely to be relatively little product innovation, but intensive process innovation. Also, equipment will be designed for a specific process step. On the other hand, the manufacture of fine and specialty chemicals might involve:

- selling into a market with low volume;
- a short product life cycle;
- a demand for a short time to market, and therefore less time is available for process development, with product and process development proceeding simultaneously.

As a result, the manufacture of fine and specialty chemicals is often carried out in multipurpose equipment, perhaps with different chemicals being manufactured in the same equipment at different times during the year. The life of the equipment might greatly exceed the life of the product.

The development of pharmaceutical products demands that high-quality products must be manufactured during the development of the process to allow safety and clinical studies to be carried out before full-scale production. Pharmaceutical production represents an extreme case of process design in which the regulatory framework controlling production makes it difficult to make process changes, even during the development stage. Even if significant improvements to processes for pharmaceuticals can be suggested, it might not be feasible to implement them, as such changes might prevent or delay the process from being licensed for production.

1.2 Formulation of Design Problems

Before a process design can be started, the design problem must be formulated. Formulation of the design problem requires a product specification. If a well-defined chemical product is to be manufactured, then the specification of the product might appear straightforward (e.g. a purity specification). However, if a specialty product is to be manufactured, it is the functional properties that are important, rather than the chemical properties, and this might require a *product design* stage in order to specify the product (Seider *et al.*, 2010; Cussler and Moggridge, 2011).

The initial statement of the design problem is often ill defined. For example, the design team could be asked to expand the production capacity of an existing plant that produces a chemical that is a precursor to a polymer product, which is also produced by the company. This results from an increase in the demand for the polymer product and the plant producing the precursor currently being operated at its maximum capacity. The design team might well be given a specification for the expansion. For example, the marketing department might assess that the market could be expanded by 30% over a two-year period, which would justify a 30% expansion in the process for the precursor. However, the 30% projection can easily be wrong. The economic environment can change, leading to the projected increase being either too large or too small. It might also be possible to sell the polymer precursor in the market to other manufacturers of the polymer and justify an expansion even larger than 30%. If the polymer precursor can be sold in the marketplace, is the current purity specification of the company suitable for the marketplace? Perhaps the marketplace demands a higher purity than the current company specification. Perhaps the current specification is acceptable, but if the specification could be improved, the product could be sold for a higher value and/or at a greater volume. An option might be to not expand the production of the polymer precursor to 30%, but instead to purchase it from the market. If it is purchased from the market, is it likely to be up to the company specifications or will it need some purification before it is suitable for the company's polymer process? How reliable will the market source be? All these uncertainties are related more to market supply and demand issues than to specific process design issues.

Closer examination of the current process design might lead to the conclusion that the capacity can be expanded by 10% with a very modest capital investment. A further increase to 20% would require a significant capital investment, but an expansion to 30% would require an extremely large capital investment. This opens up further options. Should the plant be expanded by 10% and a market source identified for the balance? Should the plant be expanded to 20% similarly? If a real expansion in the marketplace is anticipated and expansion to 30% would be very expensive, why not be more aggressive and, instead of expanding the existing process, build an entirely new process? If a new process is to be built, then what should be the process technology? New process technology might have been developed since the original plant was built that enables the same product to be manufactured at a much lower cost. If a new process is to be built, where should it be built? It might make more sense to build it in another country that would allow lower operating costs, and the product could be shipped back to be fed to the existing polymer process. At the same time, this might stimulate the development of new markets in other countries, in which case, what should be the capacity of the new plant?

Thus, from the initial ill-defined problem, the design team must create a series of very specific options and these should then be compared on the basis of a common set of assumptions regarding, for example, raw materials and product prices. Having specified an option, this gives the design team a well-defined problem to which the methods of engineering and economic analysis can be applied.

In examining a design option, the design team should start out by examining the problem at the highest level, in terms of its feasibility with the minimum of detail to ensure the design option is worth progressing (Douglas, 1985). Is there a large difference between the value of the product and the cost of the raw materials? If the overall feasibility looks attractive, then more detail can be added, the option re-evaluated, further detail added, and so on. Byproducts might play a particularly important role in the economics. It might be that the current process produces some byproducts that can be sold in small quantities to the market. However, as the process is expanded, there might be market constraints for the new scale of production. If the byproducts cannot be sold, how does this affect the economics?

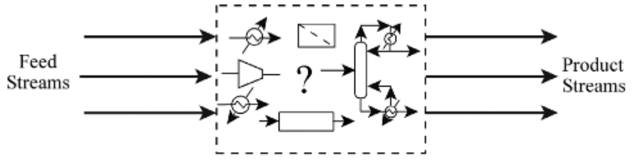
In summary, the original problem posed to process design teams is often ill defined, even though it might appear to be well defined in the original design specification. The design team must then formulate a series of plausible design options to be screened by the methods of engineering and economic analysis.

These design options are formulated into very specific design problems. In this way, the design team turns the ill-defined problem into a series of well-defined design options for analysis.

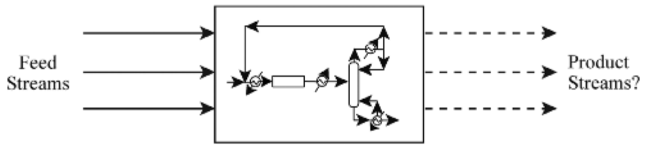
1.3 Synthesis and Simulation

In a chemical process, the transformation of raw materials into desired chemical 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 or enlargement for solids. Once individual steps have been selected, they must be interconnected to carry out the overall transformation (Figure 1.2a). 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 process that achieves the required overall transformation. A *flowsheet* or *process flow diagram* (PFD) is a 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 that attempts to predict how the process would behave if it was constructed (Figure 1.2b). Material and energy balances can be formulated to give better definition to the inner workings of the process and a more detailed process design can be developed. Having created a model of the process, the flowrates, compositions, temperatures and pressures of the feeds can be assumed. The simulation model then predicts the flowrates, compositions, temperatures, pressures and properties of the products. It also allows the individual items of equipment in the process to be sized and predicts, for example, how much raw material is being used or how much energy is being consumed. The performance of the design can then be evaluated.



(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 1.2

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

1) *Accuracy of design calculations.* A simulation adds more detail once a design has been synthesized. The design calculations for this will most often be carried out in a general purpose simulation software package and solved to a high level of precision. However, a high level of precision cannot usually be justified in terms of the operation of the plant after it has been built. The plant will almost never work precisely at its original design flowrates, temperatures, pressures and compositions. This might be because the raw materials are slightly different from what is assumed in the design. The physical properties assumed in the calculations might have been erroneous in some way, or operation at the original design conditions might create corrosion or fouling problems, or perhaps the plant cannot be controlled adequately at the original conditions, and so on, for a multitude of other possible reasons. The instrumentation on the plant will not be able to measure the flowrates, temperatures, pressures and compositions as accurately as the calculations performed. High precision might be required in the calculations for certain specific parts of the design. For example, a polymer precursor might need certain impurities to be very tightly controlled, perhaps down to the level of parts per million, or it might be that some contaminant in a waste stream might be exceptionally environmentally harmful and must be extremely well defined in the design calculations.

   Even though a high level of precision cannot be justified in many cases in terms of the plant operation, the design calculations will normally be carried out to a reasonably high level of precision. The value of precision in design calculations is that the consistency of the calculations can be checked to allow errors or poor assumptions to be identified. It also allows the design options to be compared on a valid like-for-like basis.

   Because of all the uncertainties in carrying out a design, the specifications are often increased beyond those indicated by the design calculations and the plant is *overdesigned*, or *contingency* is added, through the application of *safety factors* to the design. For example, the designer might calculate the number of distillation plates required for a distillation separation using elaborate calculations to a high degree of precision, only to add an arbitrary extra 10% to the number of plates for contingency. This allows for the feed to the unit not being exactly as specified, errors in the physical properties, upset conditions in the plant, control requirements, and so on. If too little contingency is added, the plant might not work. If too much contingency is added, the plant will not only be unnecessarily expensive but too much overdesign might make the plant difficult to operate and might lead to a less efficient plant. For example, the designer might calculate the size of a heat exchanger and then add in a large contingency and significantly oversize the heat exchanger. The lower fluid velocities encountered by the oversized heat exchanger can cause it to have a poorer performance and to foul-up more readily than a smaller heat exchanger.

Too little overdesign might lead to the plant not working. Too much overdesign will lead to the plant becoming unnecessarily expensive, and perhaps difficult to operate and less efficient. A balance must be made between different risks.

2) *Physical properties in process design.* Almost all design calculations require physical properties of the solids, liquids and gases being fed, processed and produced. Physical properties can be critical to obtaining meaningful, economic and safe designs. When carrying out calculations in computer software packages there is most often a choice to be made for the physical property correlations and data. However, if poor decisions are made by the designer regarding physical properties, the design calculations can be meaningless or even dangerous, even though the calculations have been performed to a high level of precision. Using physical property correlations outside the ranges of conditions for which they were intended can be an equally serious problem. Appendix A discusses physical properties in process design in more detail.

3) *Evaluation of performance.* 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 to maximize the *sustainability* of industrial activity. Maximizing sustainability requires that industrial systems should strive to satisfy human needs in an economically viable, environmentally benign and socially beneficial way (Azapagic, 2014). For chemical process design, this means that processes should make use of materials of construction that deplete the resource as little as practicable. Process raw materials should be used as efficiently as is economic and practicable, both to prevent the production of waste that can be environmentally harmful and to preserve the reserves of manufacturing raw materials as much as possible. Processes should use as little energy as is economic and practicable, both to prevent the build-up of carbon dioxide in the atmosphere from burning fossil fuels and to preserve the reserves of fossil fuels. Water must also be consumed in sustainable quantities that do not cause deterioration in the quality of the water source and the long-term quantity of the reserves. Aqueous and atmospheric emissions must not be environmentally harmful and solid waste to landfill must be avoided. The boundary of consideration should go beyond the immediate boundary of the manufacturing facility to maximize the benefit to society to avoid adverse health effects, unnecessarily high burdens on transportation, odour, noise nuisances, and so on.

The process must also meet required health and safety criteria. Start-up, emergency shutdown and ease of control are other important factors. Flexibility, that is, the ability to operate under different conditions, such as differences in feedstock and product specification, may be important. Availability, that is, the portion of the total time that the process meets its production requirements, might also be critically important. Uncertainty in the design, for example, resulting from poor design data, or uncertainty in the economic data might guide the design away from certain options. Some of these factors, such as economic performance, can be readily quantified; others, such as safety, often cannot. Evaluation of the factors that are not readily quantifiable, the intangibles, requires the judgment of the design team.

4) *Materials of construction.* Choice of materials of construction affects both the mechanical design and the capital cost of equipment. Many factors enter into the choice of the materials of construction. Among the most important are (see Appendix B):

- mechanical properties (particularly yield and tensile strength, compressive strength, ductility, toughness, hardness, fatigue limit and creep resistance);
- effect of temperature on mechanical properties (both low and high temperatures),
- ease of fabrication (machining, welding, and so on);
- corrosion resistance;
- availability of standard equipment in the material;
- cost (e.g. if materials of construction are particularly expensive, it might be desirable to use a cheaper material together with a lining on the process side to reduce the cost).

Estimation of the capital cost and preliminary specification of equipment for the evaluation of performance requires decisions to be made regarding the materials of construction. The discussion of the more commonly used materials of construction is given in Appendix B.

5) *Process safety.* When evaluating a process design, process safety should be the prime consideration. Safety considerations must not be left until the design has been completed. Safety systems need to be added to the design later for the relief of overpressure, to trip the process under dangerous conditions, etc. However, by far the largest impact on process safety can be made early in the design through measures to make the design *inherently safer*. This will be discussed in detail in Chapter 28. Inherently safer design means avoiding the need for hazardous materials if possible, or using less of them, or using them at lower temperatures and pressures or diluting them with inert materials. One of the principal approaches to making a process inherently safer is to limit the inventory of hazardous material. The inventories to be avoided most of all are flashing flammable or toxic liquids, that is, liquids under pressure above their atmospheric boiling points (see Chapter 28).

6) *Optimization.* Once the basic performance of the design has been evaluated, changes can be made to improve the performance; the process is *optimized*. These changes might involve the synthesis of alternative structures, that is, *structural optimization*. Thus, the process is simulated and evaluated again, and so on, optimizing the structure. Each structure can be subjected to *parameter optimization* by changing operating conditions within that structure. This is illustrated in Figure 1.3.

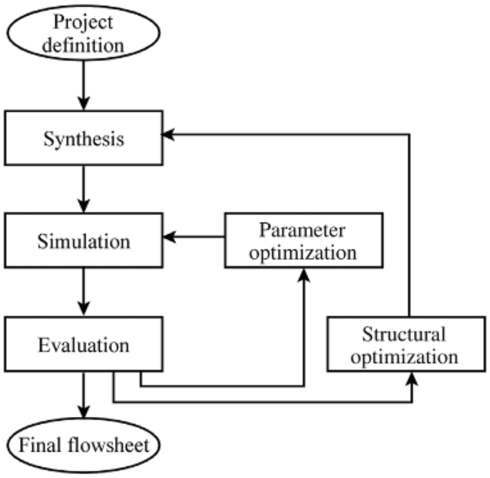


Figure 1.3

Optimization can be carried out as structural or parameter optimization to improve the evaluation of the design.

From the project definition an initial design is synthesized. This can then be simulated and evaluated. Once evaluated, the design can be optimized in a parameter optimization through changing the continuous parameters of flowrate, composition, temperature and pressure to improve the evaluation. However, this parameter optimization only optimizes the initial design configuration, which might not be an optimal configuration. So the design team might return to the synthesis stage to explore other configurations in a structural optimization. Also, if the parameter optimization adjusts the settings of the conditions to be significantly different from the original assumptions, then the design team might return to the synthesis stage to consider other configurations in the structural optimization. The different ways this design process can be followed will be considered later in this chapter.

7) *Keeping design options open.* To develop a design concept requires design options to be first generated and then evaluated. There is a temptation to carry out preliminary evaluation early in the development of a design and eliminate options early that initially appear to be unattractive. However, this temptation must be avoided. In the early stages of a design the uncertainties in the evaluation are often too serious for early elimination of options, unless it is absolutely clear that a design option is not viable. Initial cost estimates can be very misleading and the full safety and environmental implications of early decisions are only clear once detail has been added. If it was possible to foresee everything that lay ahead, decisions made early might well be different. There is a danger in focusing on one option without rechecking the assumptions later for validity when more information is available. The design team must not be boxed in early by preconceived ideas. This means that design options should be left open as long as practicable until it is clear that options can be closed down. All options should be considered, even if they appear unappealing at first.

1.4 The Hierarchy of Chemical Process Design and Integration

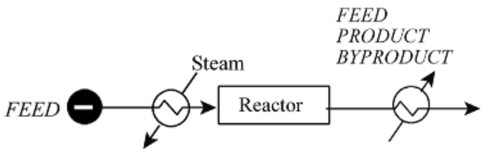
Consider the process illustrated in Figure 1.4 (Smith and Linnhoff, 1988). The process requires a reactor to transform the *FEED* into *PRODUCT* (Figure 1.4a). Unfortunately, not all the *FEED* reacts. Also, part of the *FEED* reacts to form *BYPRODUCT* instead of the desired *PRODUCT*. A separation system is needed to isolate the *PRODUCT* at the required purity. Figure 1.4b shows one possible separation system consisting of two distillation columns. The unreacted *FEED* in Figure 1.4b is recycled and the *PRODUCT* and *BYPRODUCT* are removed from the process. Figure 1.4b shows a flowsheet where 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 heat should be recovered. Thus, *heat integration* is carried out to exchange heat between those streams that need to be cooled and those that need to be heated. Figure 1.5 (Smith and Linnhoff, 1988) shows two possible designs for the *heat exchanger network*, but many other heat integration arrangements are possible.

The flowsheets shown in Figure 1.5 feature the same reactor design. It could be useful to explore the changes in reactor design. For example, the size of the reactor could be increased to increase the amount of *FEED* that reacts (Smith and Linnhoff, 1988). Now there is not only much less *FEED* in the reactor effluent but also more *PRODUCT* and *BYPRODUCT*. However, the increase in *BYPRODUCT* is larger than the increase in *PRODUCT*. Thus, although the reactor has the same three components in its effluent as the reactor in Figure 1.4a, 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 Figures 1.4 and 1.5 is now appropriate. Figure 1.6 shows a possible alternative. This also uses two distillation columns, but the separations are carried out in a different order.

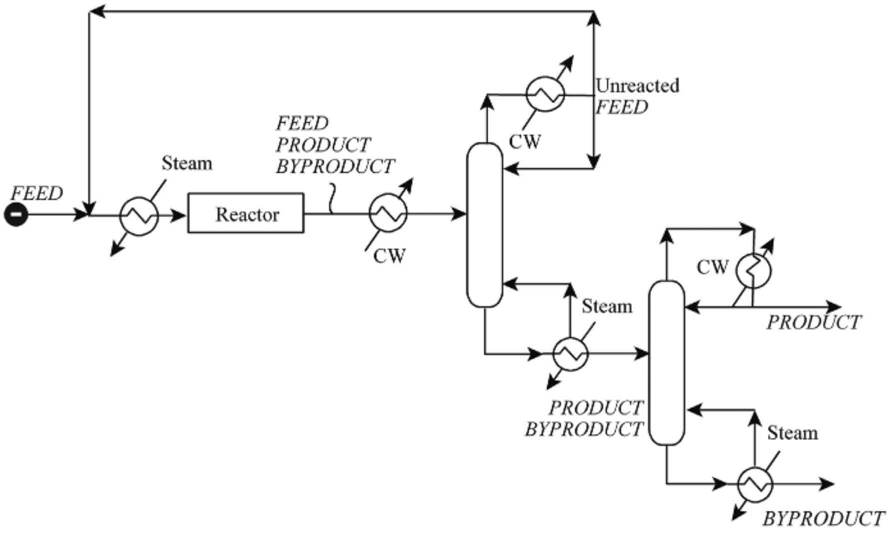
Figure 1.6 shows a flowsheet without any heat integration for the different reactor and separation system. As before, this is probably too inefficient in the use of energy, and heat integration schemes can be explored. Figure 1.7 (Smith and Linnhoff, 1988) shows two of the many possible flowsheets involving heat recovery.

Different complete flowsheets can be evaluated by simulation and costing. On this basis, the flowsheet in Figure 1.5b might be more promising than the flowsheets in Figures 1.5a and 1.7a and b. However, the best flowsheet cannot be identified without first optimizing the operating conditions for each. The flowsheet in Figure 1.7b might have greater scope for improvement than that in Figure 1.5b, and so on.

Thus, the complexity of chemical process synthesis is twofold. First, can all possible structures be identified? It might be considered that all the structural options can be found by inspection, at least all of the significant ones. The fact that



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



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

Figure 1.4

Process design starts with the reactor. The reactor design dictates the separation and recycle problem. (Reproduced from Smith R and Linnhoff B, 1998, *Trans IChemE ChERD*, **66**: 195 by permission of the Institution of Chemical Engineers.)

even long-established processes are still being improved bears evidence to just how difficult this is. Second, can each structure be optimized 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 the operating conditions for a multitude of structural options must be simulated and optimized. At first sight, this appears to be an overwhelmingly complex problem.

It is helpful when developing a methodology if there is a clear picture of the nature of the problem. If the process requires a reactor, this is where the design starts. This is likely to be the only place in the process where raw material components are converted into components for the 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 the reactor design. The reactor and separation and recycle system designs together define the process for heating and cooling duties. Thus, the heat exchanger network design comes next. Those heating and cooling duties that cannot be satisfied by heat recovery dictate the need for external heating and cooling *utilities* (furnace heating, use of steam, steam generation, cooling water, air cooling or refrigeration). Thus, utility selection and design follows the design of the heat recovery system. The selection and design of the utilities is made more complex by the fact that the process will most likely operate within the context of a site comprising a number of different processes that are all connected to a common utility system. The process and the utility system will both need water, for example, for steam generation, and will also produce aqueous effluents that will have to be brought to a suitable quality for discharge. Thus, the design of the water and aqueous effluent treatment system comes last. Again, the water and effluent treatment system must be considered at the site level as well as the process level.

This hierarchy can be represented symbolically by the layers of the "onion diagram" shown in Figure 1.8 (Linnhoff *et al.*, 1982). The diagram emphasizes the sequential, or hierarchical, nature of process design. Other ways to represent the hierarchy have also been suggested (Douglas, 1985).

Some processes do not require a reactor, for example, some processes just involve separation. Here, the design starts with the separation system and moves outward to the heat exchanger network, utilities, and so on. However, the same basic hierarchy prevails.

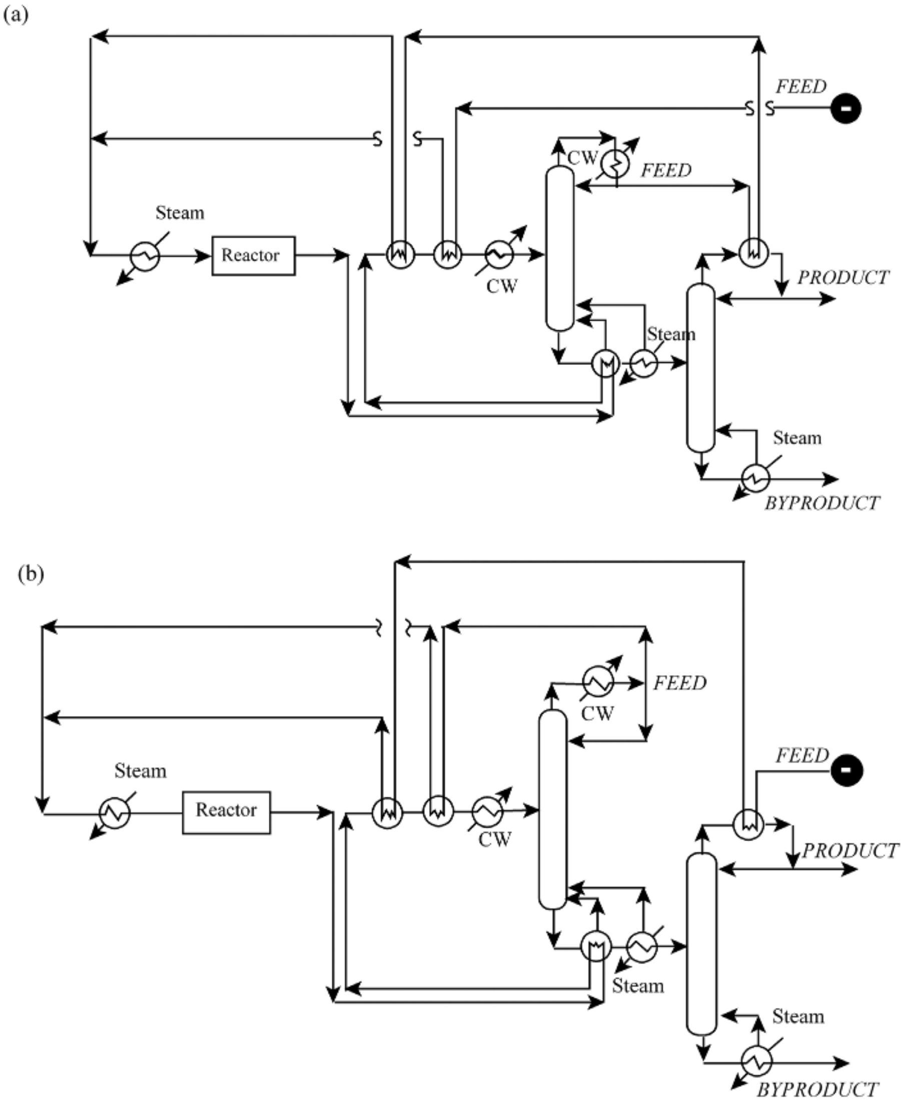


Figure 1.5

For a given reactor and separator design there are different possibilities for heat integration. (Reproduced from Smith R and Linnhoff B, 1998, *Trans IChemE ChERD*, **66**: 195 by permission of the Institution of Chemical Engineers.)

The synthesis of the correct structure and the optimization of parameters in the design of the reaction and separation systems are often the 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 model. For example, it is not possible to assess which is better, the basic scheme from Figure 1.4b or that from Figure 1.6, without fully evaluating all possible designs, such as those shown in Figures 1.5a and b and 1.7a and b, all completed, including utilities. Such a complete search is normally too time-consuming to be practical.

Later, in Chapter 17, an approach will be 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”.

1.5 Continuous and Batch Processes

When considering the processes in Figures 1.4 to 1.6, an implicit assumption was made that the processes operated continuously. However, not all processes operate continuously. In a *batch* process, the main steps operate discontinuously. In contrast with a continuous process, a batch process does not deliver its product continuously but in discrete amounts. This means that heat, mass, temperature, concentration and other properties vary with time. In practice, most batch processes are made up of a series of batch and *semi-continuous* steps. A semi-continuous step runs continuously with periodic start-ups and shutdowns.

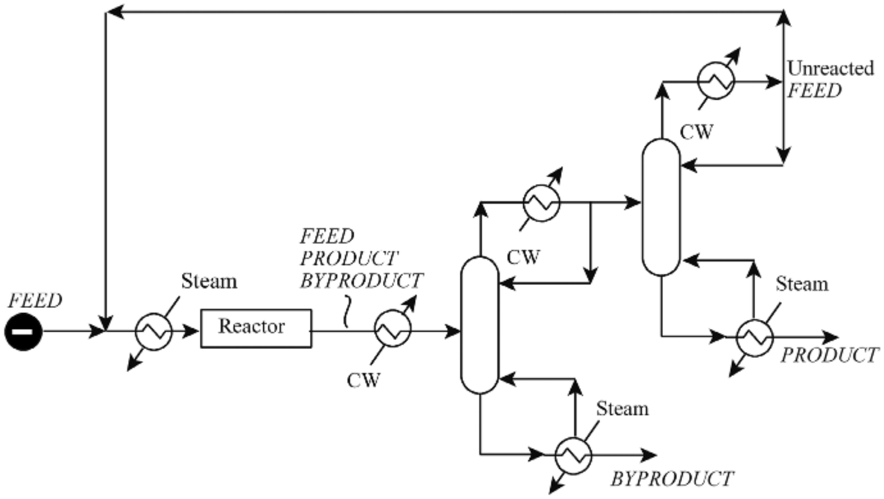


Figure 1.6

Changing the reactor dictates a different separation and recycle problem. (Reproduced from Smith R and Linnhoff B, 1998, *Trans IChemE ChERD*, **66**: 195 by permission of the Institution of Chemical Engineers.)

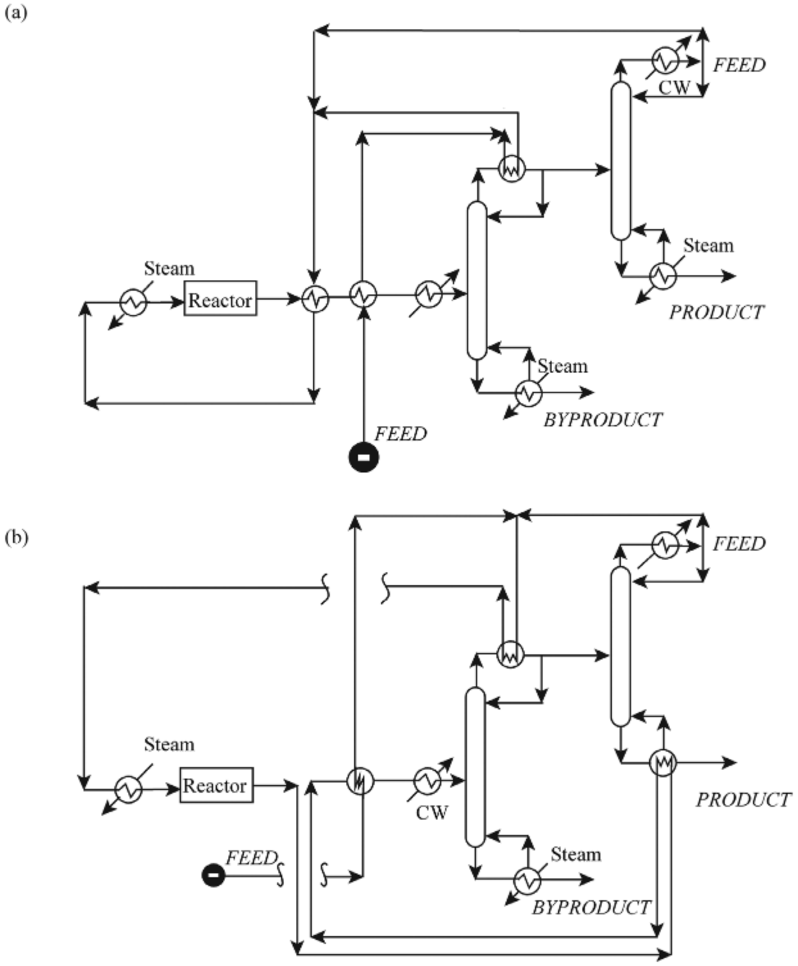


Figure 1.7

A different reactor design not only leads to a different separation system but additional possibilities for heat integration. (Reproduced from Smith R and Linnhoff B, 1998, *Trans IChemE ChERD*, **66**: 195 by permission of the Institution of Chemical Engineers.)

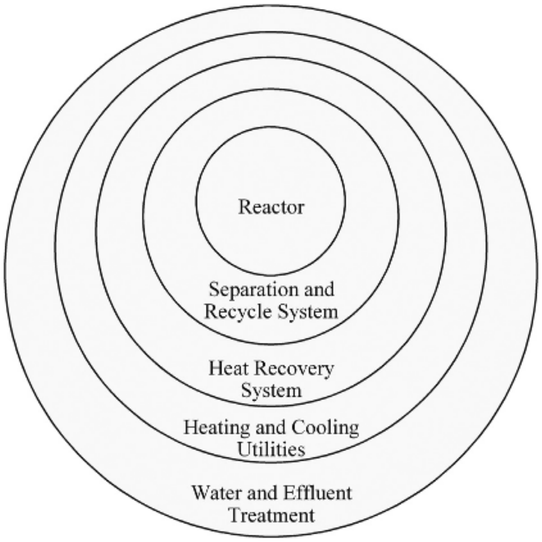


Figure 1.8

The onion model of process design. A reactor is needed before the separation and recycle system can be designed, and so on.

Consider the simple process shown in Figure 1.9. Feed material is withdrawn from storage using a pump. The feed material is preheated in a heat exchanger before being fed to a batch reactor. Once the reactor is full, further heating takes place inside the reactor by passing steam into the reactor jacket before the reaction proceeds. During the later stages of the reaction, cooling water is applied to the reactor jacket. Once the reaction is complete, the reactor product is withdrawn using a pump. The reactor product is cooled in a heat exchanger before going to storage.

The first two steps, pumping for reactor filling and feed preheating, are both semi-continuous. The heating inside the reactor, the reaction itself and the cooling using the reactor jacket are all batch. The pumping to empty the reactor and the product-cooling step are again semi-continuous.

The hierarchy in batch process design is no different from that in continuous processes and the hierarchy illustrated in Figure 1.8 prevails for batch processes also. However, the time dimension brings constraints that do not present a problem in the design of continuous processes. For example, heat recovery might be considered for the process in Figure 1.9. The reactor effluent (which requires cooling) could be used to preheat the incoming feed to the reactor (which requires heating). Unfortunately, even if the reactor effluent is at a high enough temperature to allow this, the reactor feeding and emptying take place at different times, meaning that this will not be possible without some way to store the heat. Such heat storage is possible but usually uneconomic, especially for small-scale processes.

If a batch process manufactures only a single product, then the equipment can be designed and optimized for that product. The dynamic nature of the process creates additional challenges for design and optimization. It might be that the optimization calls for variations in the conditions during the batch through time, according to some *profile*. For example, the temperature in a batch reactor might need to be increased or decreased as the batch progresses.

Multiproduct batch processes, with a number of different products manufactured in the same equipment, present even bigger challenges for design and optimization (Biegler, Grossman and Westerberg, 1997). Different products will demand different designs, different operating conditions and, perhaps, different trajectories for the operating conditions through time. The design of equipment for multiproduct plants will thus require a compromise to be made across the requirements of a number of different products. The more flexible the equipment and the configuration of the equipment, the more it will be able to adapt to the optimum requirements of each product.

Batch processes:

- are economical for small volumes;
- are flexible in accommodating changes in product formulation;
- are flexible in changing the production rate by changing the number of batches made in any period of time;

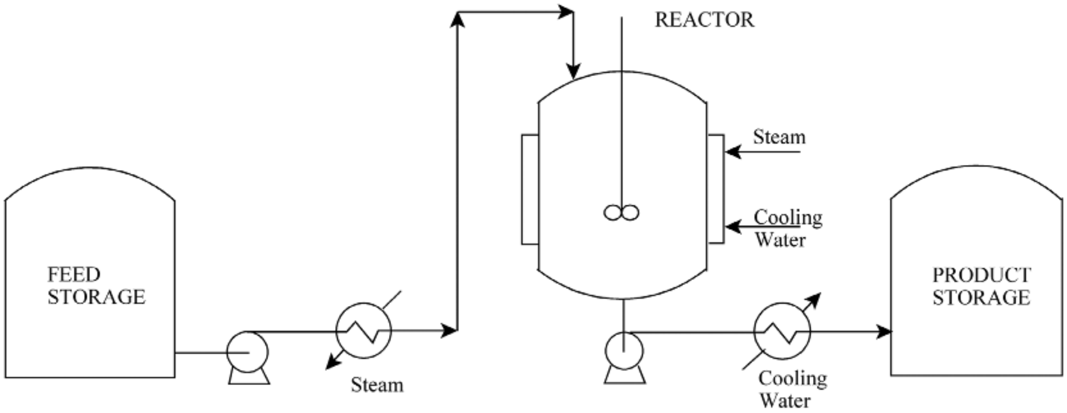


Figure 1.9

A simple batch process.

- allow the use of standardized multipurpose equipment for the production of a variety of products from the same plant;
- are best if equipment needs regular cleaning because of fouling or needs regular sterilization;
- are amenable to direct scale-up from the laboratory and
- allow product identification. Each batch of product can be clearly identified in terms of when it was manufactured, the feeds involved and conditions of processing. This is particularly important in industries such as pharmaceuticals and foodstuffs. If a problem arises with a particular batch, then all the products from that batch can be identified and withdrawn from the market. Otherwise, all the products available in the market would have to be withdrawn.

One of the major problems with batch processing is batch-to-batch conformity. Minor changes to the operation can mean slight changes in the product from batch to batch. Fine and specialty chemicals are usually manufactured in batch processes. However, these products often have very tight tolerances for impurities in the final product and demand batch-to-batch variation to be minimized.

Batch processes will be considered in more detail in Chapter 16.

1.6 New Design and Retrofit

There are two situations that can be encountered in process design. The first is in the design of *new plant* or *grassroot* design. In the second, the design is carried out to modify an existing plant in *retrofit* or *revamp*. The motivation to retrofit an existing plant could be, for example, to increase capacity, allow for different feed or product specifications, reduce operating costs, improve safety or reduce environmental emissions. One of the most common motivations is to increase capacity. When carrying out a retrofit, whatever the motivation, it is desirable to try and make as effective use as possible of the existing equipment. The basic problem with this is that the design of the existing equipment might not be ideally suited to the new role that it will be put to. On the other hand, if equipment is reused, it will avoid unnecessary investment in new equipment, even if it is not ideally suited to the new duty.

When carrying out a retrofit, the connections between the items of equipment can be reconfigured, perhaps adding new equipment where necessary. Alternatively, if the existing equipment differs significantly from what is required in the retrofit, then in addition to reconfiguring the connections between the equipment, the equipment itself can be modified. Generally, the fewer the modifications to both the connections and the equipment, the better.

The most straightforward design situations are those of grassroot design as it has the most freedom to choose the design options and the size of equipment. In retrofit, the design must try to work within the constraints of existing equipment. Because of this, the ultimate goal of the retrofit design is often not clear. For example, a design objective might be given to increase the capacity of a plant by 50%. At the existing capacity limit of the plant, at least one item of equipment must be at its maximum capacity. Most items of equipment are likely to be below their maximum capacity. The differences in the spare capacity of different items of equipment in the existing design arises from different design allowances (or *contingency*) in the original design, changes to the operation of the plant relative to the original design, errors in the original design data, and so on. An item of equipment at its maximum capacity is the *bottleneck* to prevent increased capacity. Thus, to overcome the bottleneck or *debottleneck*, the item of equipment is modified, or replaced with new equipment with increased capacity, or a new item is placed in parallel or series with the existing item, or the connections between existing equipment are reconfigured, or a combination of all these actions is taken. As the capacity of the plant is increased, different items of equipment will reach their maximum capacity. Thus, there will be thresholds in the plant capacity created by the limits in different items of equipment. All equipment with capacity less than the threshold must be modified in some way, or the plant reconfigured, to overcome the threshold. To overcome each threshold requires capital investment. As capacity is increased from the existing limit, ultimately it is likely that it will be prohibitive for the investment to overcome one of the design thresholds. This is likely to become the design limit, as opposed to the original remit of a 50% increase in capacity in the example.

Another important issue in retrofit is the downtime required to make the modifications. The cost of lost production while the plant is shut down to be modified can be prohibitively expensive. Thus, one of the objectives for retrofit is to design modifications that require only a short shutdown. This often means designing modifications that allow the bulk of the work to be carried out while the process is still in operation. For example, new equipment can be installed with final piping connections made when the process is shut down. Decisions whether to replace a major process component completely, or to supplement with a new component working in series or parallel with the existing component, can be critical to the downtime required for retrofit.

1.7 Reliability, Availability and Maintainability

As already discussed, *availability* is often an important issue in process design. Unless the plant is operating in its intended way, it is not productive. Availability measures the portion of the total time that the process meets its production requirements. Availability is related to *reliability* and *maintainability*. *Reliability* is the probability of survival after the unit/system operates for a certain period of time (e.g. a unit has a 95% probability of survival after 8000 hours). Reliability defines the failure frequency and determines the *uptime* patterns. *Maintainability* describes how long it takes for the unit/system to be repaired, which determines the *downtime* patterns. Availability measures the percentage of uptime the process operates at its production requirements over the time horizon, and is determined by reliability and maintainability.

Availability can be improved in many ways. Maintenance policy has a direct influence. *Preventive maintenance* can be used to prevent unnecessary breakdowns. *Condition monitoring* of equipment using techniques such as monitoring vibration of rotating equipment like compressors can be used to detect mechanical problems early, and again prevent unnecessary breakdowns. In design, using *standby* components (sometimes referred to as *spare* or *redundant* components) is a common way to increase system availability. Instead of having one item of equipment on line and vulnerable to breakdown, there may be two, with one on-line and one off-line. These two items of equipment can be sized and operated in many ways:

- 2 × 100% one on-line, one off-line switched off;
- 2 × 100% one on-line, one off-line idling;
- 2 × 50% both on-line, with system capacity reduced to 50% if one fails;
- 2 × 75% both on-line operating at 2/3 capacity when both operating, but with system capacity 75% if one fails;
- and so on.

Over-sizing equipment, particularly rotating equipment like pumps and compressors, can make it more reliable in some cases. Determining the optimum policy for standby equipment involves complex trade-offs that need to consider capital cost, operating cost, maintenance costs and reliability.

1.8 Process Control

Once the basic process configuration has been fixed, a *control system* must be added. The control system compensates for the influence of external *disturbances* such as changes in feed flowrate, feed conditions, feed costs, product demand, product specifications, product prices, ambient temperature, and so on. Ensuring safe operation is the most important task of a control system. This is achieved by monitoring the process conditions and maintaining them within safe operating limits. While maintaining the operation within safe operating limits, the control system should optimize the process performance under the influence of external disturbances. This involves maintaining product specifications, meeting production targets and making efficient use of raw materials and utilities.

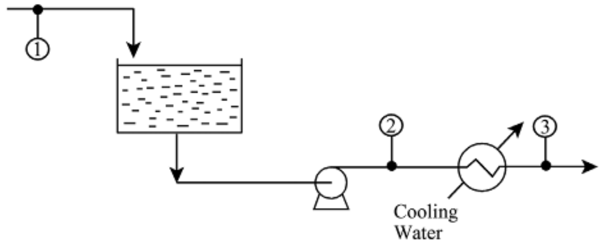
A control mechanism is introduced that makes changes to the process in order to cancel out the negative impact of disturbances. In order to achieve this, instruments must be installed to measure the operational performance of the plant. These *measured variables* could include temperature, pressure, flowrate, composition, level, pH, density and particle size. *Primary measurements* may be made to directly represent the control objectives (e.g. measuring the composition that needs to be controlled). If the control objectives are not measurable, then *secondary measurements* of other variables must be made and these secondary measurements related to the control objective. Having measured the variables that need to be controlled, other variables need to be *manipulated* in order to achieve the control objectives. A control system is then designed that responds to variations in the measured variables and manipulates other variables to control the process.

Having designed a process configuration for a continuous process and having optimized it to achieve some objective (e.g. maximize profit) at steady state, is the influence of the control system likely to render the previously optimized process to now be nonoptimal? Even for a continuous process, the process is always likely to be moving from one state to another in response to the influence of disturbances and control objectives. In the steady-state design and optimization of continuous processes, these different states can be allowed for by considering *multiple operating cases*. Each operating case is assumed to operate for a certain proportion of the year. The contribution of the operating case to the overall steady-state design and optimization is weighted according to the proportion of the time under which the plant operates at that state.

While this takes some account of operation under different conditions, it does not account for the dynamic transition from one state to another. Are these transitory states likely to have a significant influence on the optimality? If the transitory states were to have a significant effect on the overall process performance in terms of the objective function being optimized, then the process design and control system design would have to be carried out simultaneously. Simultaneous design of the process and the control system presents an extremely complex problem. It is interesting to note that where steady-state optimization for continuous processes has been compared with simultaneous optimization of the process and control system, the two process designs have been found to be almost identical (Bansal *et al.*, 2000a, 2000b; Kookos and Perkins, 2001).

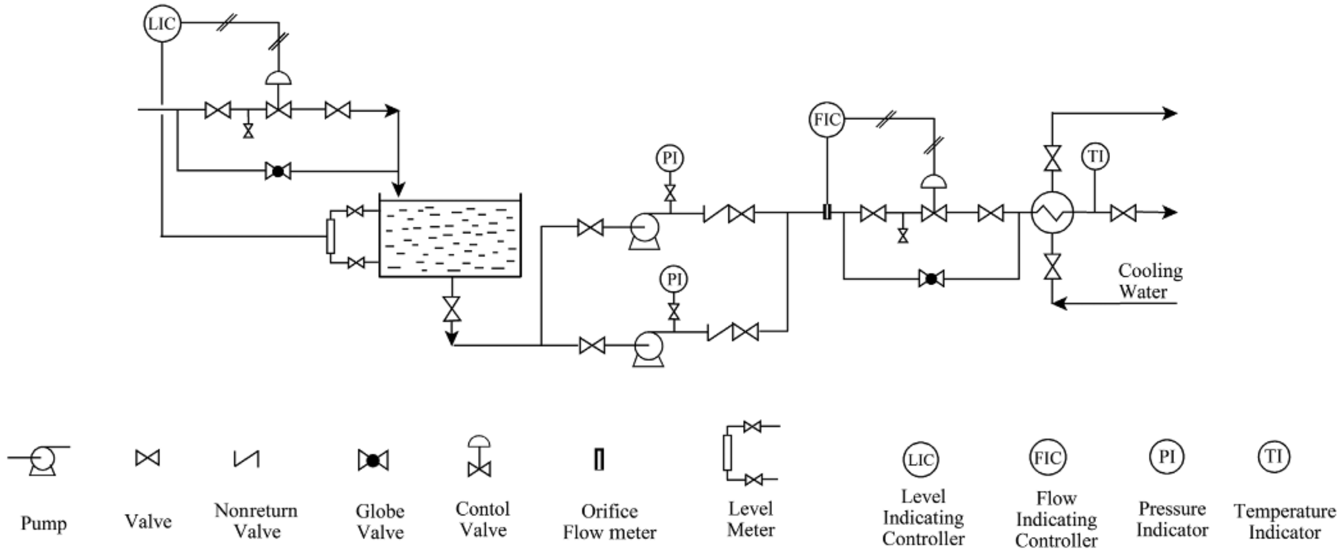
Industrial practice is to first design and optimize the process configuration (taking into account multiple states, if necessary) and then to add the control system. However, there is no guarantee that design decisions made on the basis of steady-state conditions will not lead to control problems once process dynamics are considered. For example, an item of equipment might be oversized for contingency, because of uncertainty in design data or future debottlenecking prospects, based on steady-state considerations. Once the process dynamics are considered, this oversized equipment might make the process difficult to control, because of the large inventory of process materials in the oversized equipment. The approach to process control should adopt an approach that considers the control of the whole process, rather than just the control of the individual process steps in isolation (Luyben, Tyreus and Luyben, 1999).

The control system arrangement is shown in the *piping and instrumentation diagram* (P & I D) for the process (Sinnott and Towler, 2009). The piping and instrumentation diagram shows all of the process equipment, piping connections, valves, pipe fittings and the control system. All equipment and connections are shown. This includes not only the main items of equipment and connections but also standby equipment, equipment and piping used for start-up, shutdown, maintenance operations and abnormal operation. Figure 1.10a illustrates a very simple *process flow diagram*. This shows only the main items of equipment and the normal process flows. The information shown on such process flow diagrams, and their style, vary according to the practice of different companies. As an example, Figure 1.10a shows the component flowrates and stream temperatures and pressures. By contrast Figure 1.10b shows the corresponding piping and instrumentation diagram. This shows all of the equipment (including the standby pump in this case), all piping connections and fittings, including



Line	1 Aqueous Recycle	2 Pump Discharge	3 Cooled Recycle
Water ($t{\cdot}h^{-1}$)	11.6	11.6	11.6
Salts ($t{\cdot}h^{-1}$)	0.37	0.37	0.37
Sulfuric Acid ($t{\cdot}h^{-1}$)	-	-	-
Total ($t{\cdot}h^{-1}$)	11.97	11.97	11.97
Temperature (°C)	60	60	30
Pressure (bar)	1.1	5.0	4.4

(a) A simple process flow diagram.



(b) Piping and instrumentation diagram.

Figure 1.10

Process flow diagrams (PFD) and piping and instrumentation diagrams (P&ID).

those used for start-up, shutdown, maintenance and abnormal operation. It also shows the layout of the control system. Additional information normally included would be identification numbers for the equipment, piping connections and control equipment. Information on materials of construction might also be included. But information on process flows and conditions would not normally be shown. As with process flow diagrams, the style of piping and instrumentation diagrams varies according to the practice of different companies.

This text will concentrate on the design and optimization of the process configuration and will not deal with process control. Process control demands expertise in different techniques and will be left to other sources of information (Luyben, Tyreus and Luyben, 1999). Thus, the text will describe how to develop a *flowsheet* or *process flow diagram*, but will not take the final step of adding the instrumentation, control and auxiliary pipes and valves required for the final engineering design in the piping and instrumentation diagram.

Batch processes are, by their nature, always in a transitory state. This requires the dynamics of the process to be optimized, and will be considered in Chapter 16. However, the control systems required to put this into practice will not be considered.

1.9 Approaches to Chemical Process Design and Integration

In broad terms, there are three approaches to chemical process design and integration:

1) *Creating 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, decisions must be made on the basis of 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 creation of the design involves making a series of best local decisions. This might be based on the use of *heuristics* or *rules of thumb* developed from experience (Douglas, 1985) or on a more systematic approach. 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 that are technically or economically redundant are not included.

There are two drawbacks to this approach:

a) Different decisions are possible at each stage of the design. To be sure that the best decisions have been made, 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) Completing and evaluating many options gives no guarantee of ultimately finding the best possible design, as the search is not exhaustive. Also, complex interactions can occur between different parts of a flowsheet. The effort to keep the system simple and not add features in the early stages of design may result in missing the benefit of interactions between different parts of the flowsheet in a more complex system.

The main advantage of this approach is that the design team can keep control of the basic decisions and interact as the design 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 superstructure.* In this approach, a *reducible* structure, known as a *superstructure*, is first created that has embedded within it all feasible process options and all feasible interconnections that are candidates for an optimal design structure. Initially, redundant features are built into the superstructure. As an example, consider Figure 1.11 (Kocis and Grossmann, 1988). This shows one possible structure of a process for the manufacture of benzene from the reaction between toluene and hydrogen. In Figure 1.11, the hydrogen enters the process with a small amount of methane as an impurity. Thus, in Figure 1.11, the option of either purifying the hydrogen feed with a membrane or of passing it directly to the process is embedded. 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

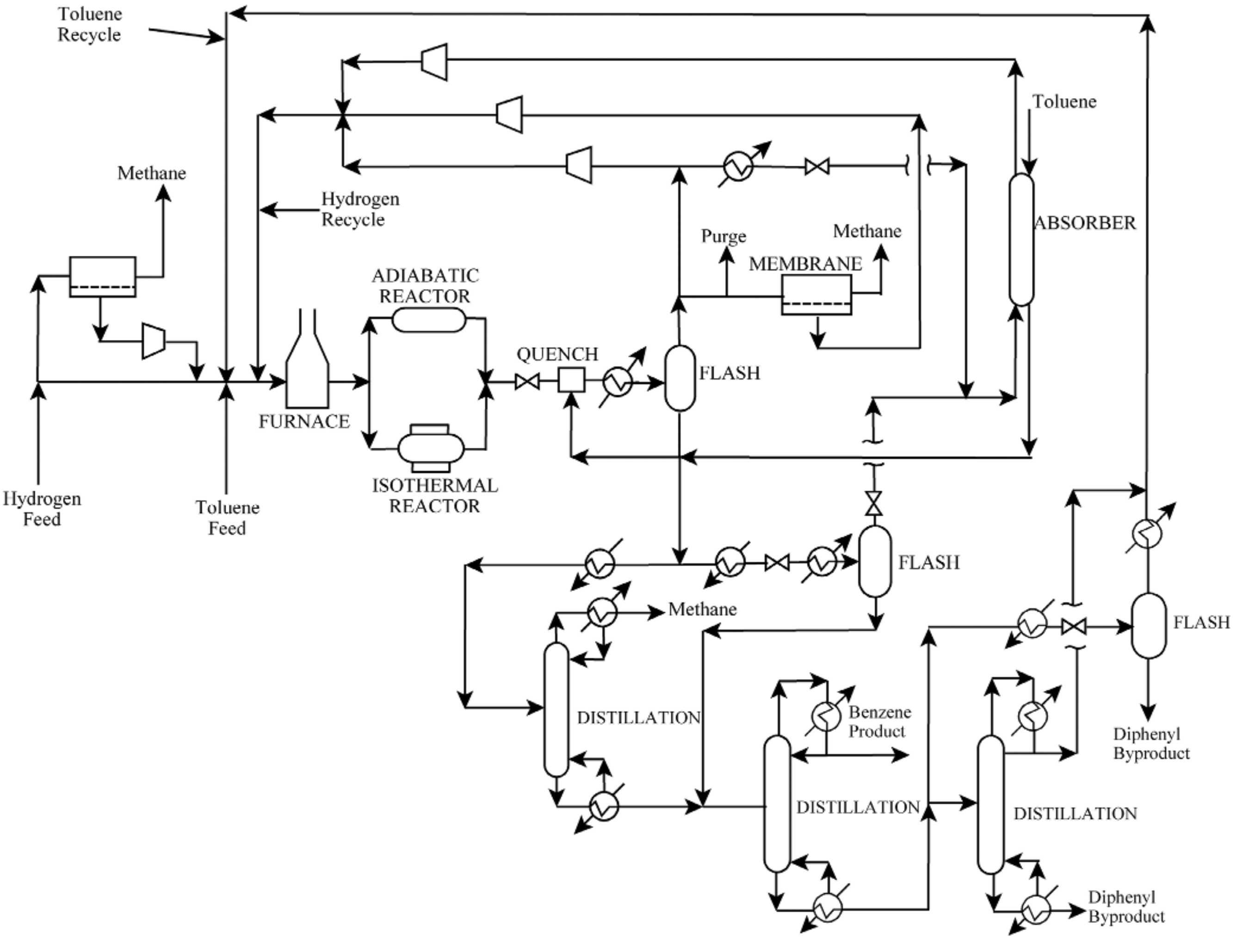


Figure 1.11

A superstructure for the manufacture of benzene from toluene and hydrogen incorporating some redundant features. (Reproduced from Kocis GR and Grossman IE, *Comp Chem Eng*, **13**: 797, with permission from Elsevier.)

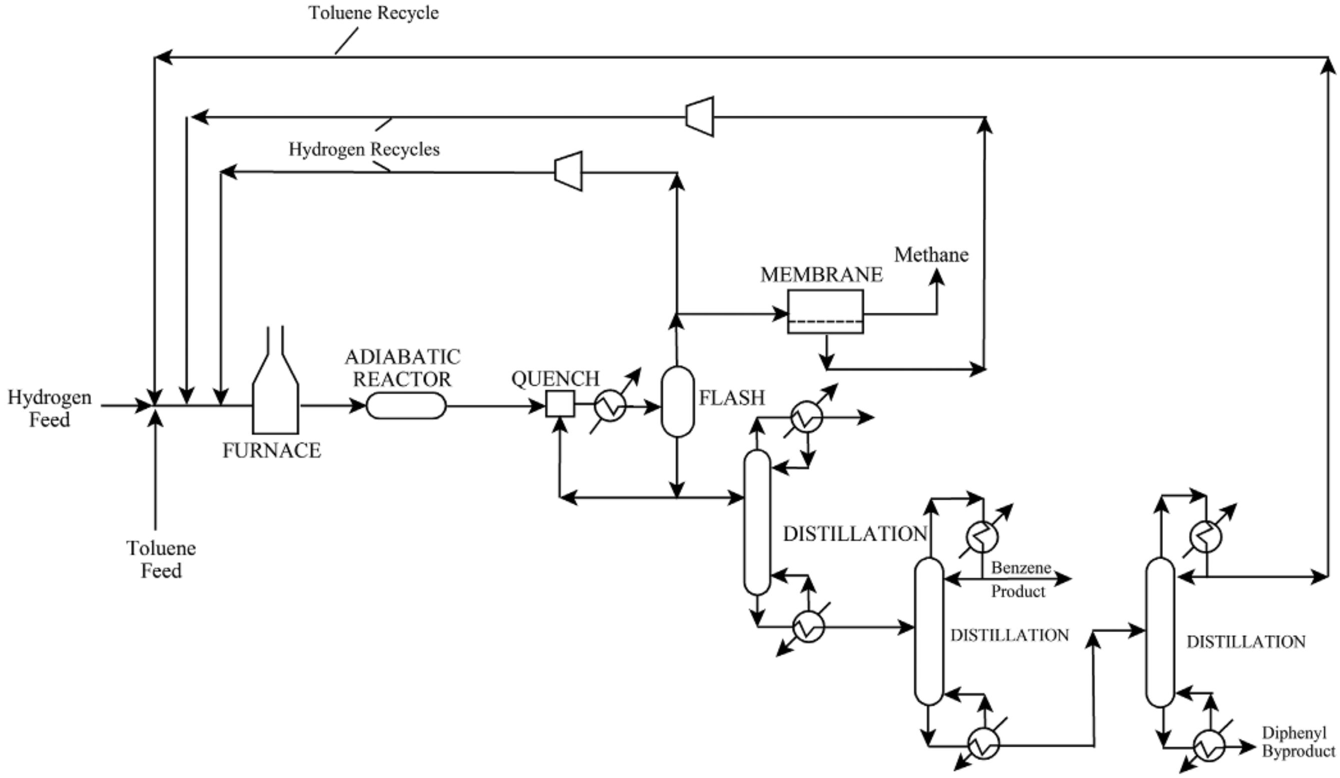


Figure 1.12

Optimization discards many structural features leaving an optimized structure. (Reproduced from Kocis GR and Grossman IE, *Comp Chem Eng*, **13**: 797, with permission from Elsevier.)

required. Then the 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 model. Some of the design features are continuous, describing the operation of each unit (e.g. flowrate, composition, temperature and pressure) and its size (e.g. volume, heat transfer area, etc.). Other features are discrete (e.g. whether a connection in the flowsheet is included or not, a membrane separator is included or not). Once the problem is formulated mathematically, its solution is carried out through the implementation of an optimization algorithm. An *objective function* is maximized or minimized (e.g. profit is maximized or cost is minimized) in a *structural and parameter* optimization. The optimization justifies the existence of structural features and deletes those features from the structure that cannot be justified economically. In this way, the structure is reduced in complexity. At the same time, the operating conditions and equipment sizes are also optimized. In effect, the discrete decision-making aspects of process design are replaced by a discrete/continuous optimization. Thus, the initial structure in Figure 1.11 is optimized to reduce the structure to the final design shown in Figure 1.12 (Kocis and Grossmann, 1988). In Figure 1.12, the membrane separator on the hydrogen feed has been removed by optimization, as has the isothermal reactor and many other features of the initial structure shown in Figure 1.11.

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 mathematical model will be extremely large and the objective function that must be optimized will be extremely irregular. The profile of the objective function can be like the terrain in a range of mountains with many peaks and valleys. If the objective function is to be maximized (e.g. maximize profit), each peak in the mountain range represents a *local optimum* in the objective function. The highest peak represents 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 the direction and an altimeter to show the 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 to fall into that might be impossible to climb out of.

Such problems can be overcome in a number of ways. The first way is by changing the model such that the solution space becomes more regular, making the optimization simpler. This most often means simplifying the mathematical model. A second way is by repeating the search many times, but starting each new search from a different initial location. A third way exploits mathematical transformations and bounding techniques for some forms of mathematical expression to allow the global optimum to be found (Floudas, 2000). A fourth way is by allowing the optimization to search the solution space so as to allow the possibility of going downhill, away from an optimum point, as well as uphill. As the search proceeds, the ability of the algorithm to move downhill must be gradually taken away. These problems will be dealt with in more detail in Chapter 3.

c) The most serious drawback of this approach is that the design engineer is removed from the decision making. Thus, the many intangibles in design, such as safety and layout, 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. The complex multiple trade-offs usually encountered in chemical process design can be handled by this approach. Also, the entire design procedure can be automated and is capable of producing designs quickly and efficiently.

3) *Creating an initial design and evolving through structural and parameter optimization.* The third approach is a variation on creating and optimizing a superstructure. In this approach, an initial design is first created. This is not necessarily intended to be an optimal design and does not necessarily have redundant features, but is simply a starting point. The initial design is then subjected to *evolution* through structural and parameter optimization, using an optimization algorithm (see Chapter 3). As with the superstructure approach, the design problem is formulated as a mathematical model. The design is then evolved one step at a time. Each step is known as a *move*. Each move in the evolution might change one of the continuous variables in the flowsheet (e.g. flowrate, composition, temperature or pressure) or might change the flowsheet structure. Changing the flowsheet structure might mean adding or deleting equipment (together with the appropriate connections), or adding new connections or deleting existing connections.

At each move, the objective function is evaluated (e.g. profit or cost). New moves are then carried out with the aim of improving the objective function. Rules must be created to specify the moves. The same structural options might be allowed as included in the superstructure approach, but in this evolutionary approach the structural moves are carried out to add or delete structural features one at a time. In addition to the structural moves, continuous moves are also carried out to optimize the flowsheet conditions.

The difficulties associated with this approach are similar to those for the creation and optimization of a superstructure:

a) The approach will fail to find the optimal structure if the structural moves have not been defined such that the sequence of moves can lead to the optimal structure from the initial design.

b) The objective function that must be optimized will be extremely irregular. Thus, again there are difficulties finding the global optimum. The optimization methods normally adopted for this approach allow the search to proceed even if the objective function deteriorates after a move. The ability of the algorithm to accept the deteriorating objective function is gradually taken away as the optimization proceeds. This approach will be dealt with in more detail in Chapter 3.

c) Again, this approach has the disadvantage that the design engineer is removed from the decision making.

In summary, the three general approaches to chemical process design have advantages and disadvantages. However, whichever is used in practice, there is no substitute for understanding the problem.

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

1.10 The Nature of Chemical Process Design and Integration – Summary

Chemical products can be divided into three broad classes: commodity, fine and specialty chemicals. Commodity chemicals are manufactured in large volumes with low added value. Fine and specialty chemicals tend to be manufactured in low volumes with high added value. The priorities in the design of processes for the manufacture of these three classes of chemical products will differ.

The original design problem posed to the design team is often ill defined, even if it appears on the surface to be well defined. The design team must formulate well-defined design options from the original ill-defined problem, and these must be compared on the basis of consistent criteria.

Design starts by synthesizing design options, followed by simulation and evaluation. The simulation allows further detail to be added to the design. Care should be taken when carrying out simulation to choose appropriate physical property correlations and data. Safety should be considered as early as possible in the development of the design to make the design inherently safe. Both structural and parameter optimization can be carried out to improve the evaluation. Design options should be left open as far as practicable to avoid potentially attractive options being eliminated inappropriately on the basis of uncertain data.

The design might be new or retrofit of an existing process. If the design is a retrofit, then one of the objectives should be to maximize the use of existing equipment, even if it is not ideally suited to its new purpose. Another objective is to minimize the downtime required to carry out the modification.

Both continuous and batch process operations can be used. Batch processes are generally preferred for small-scale and specialty chemicals production.

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 the desired chemical products. The reactor design dictates the separation and recycle problem. Together, the reactor design and separation and recycle dictate the heating and cooling duties for the heat exchanger network. Those duties that cannot be satisfied by heat recovery dictate the need for external heating and cooling utilities. The process and the utility system both have a demand for water and create aqueous effluents, giving rise to the water system. This hierarchy is represented by the layers in the "onion diagram" of Figure 1.8. Both continuous and batch process design follow this hierarchy, even though the time dimension in batch processes brings additional constraints in process design.

There are three general approaches to chemical process design:

- creating an irreducible structure;
- creating and optimizing a superstructure;
- creating an initial design and evolving through structural and parameter optimization.

Each of these approaches have advantages and disadvantages.

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