1 Integrated Process Design

1.1 Motivation and Objectives

1.1.1 Innovation Through a Systematic Approach

Innovation is the key issue in chemical process industries in today's globalization environment, as the best means to achieve high efficiency and competitiveness with sustainable development. The job of a designer is becoming increasingly challenging. He/she has to take into account a large number of constraints of technical, economical and social nature, often contradictory. For example, the discovery of a new catalyst could make profitable cheaper raw materials, but needs much higher operating temperatures and pressures. To avoid the formation of byproducts lower conversion should be maintained, implying more energy and equipment costs. Although attractive, the process seems more expensive. However, higher temperature can give better opportunities for energy saving by process integration. In addition, more compact and efficient equipment can be designed by applying the principles of process synthesis and intensification. In the end, the integrated conceptual design may reveal a simpler flowsheet with lower energy consumption and equipment costs.

The above example is typical. Modern process design consists of the optimal combination of technical, economic, ecological and social aspects in highly *integrated processes*. The conceptual approach implies the availability of effective cost-optimization design methods aided by powerful computer-simulation tools.

Creativity is a major issue in process design. This is not a matter only of engineering experience, but above all of adopting the approach of *process systems*. This consists of a systemic viewpoint in problem analysis supported by systematic methods in process design.

A systematic and systems approach has at least two merits:

1. Provides guidance in assessing firstly the *feasibility* of the process design as a whole, as well as its flexibility in operation, before more detailed design of components.

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2. Generates not only one supposed optimal solution, but several good *alternatives* corresponding to different *design decisions*. A remarkable feature of the systemic design is that quasioptimal targets may be set well ahead detailed sizing of equipment. In this way, the efficiency of the whole engineering work may improve dramatically by avoiding costly structural modifications in later stages.

The motivation of this book consists of using a wide range of case studies to teach generic creative issues, but incorporated in the framework of a technology of industrial significance. Computer simulation is used intensively to investigate the feasibility and support design decisions, as well as for sizing and optimization. Particular emphasis is placed on thermodynamic modeling as a fundamental tool for analysis of reactions and separations. Most of the case studies make use of chemical reactor design by kinetic modeling.

A distinctive feature of this book is the *integration of design and control* as the current challenge in process design. This is required by higher flexibility and responsiveness of large-scale continuous processes, as well as by the optimal operation of batchwise and cyclic processes for high-value products.

The case studies cover key applications in chemical process industries, from petrochemistry to polymers and biofuels. The selection of processes was confronted with the problem of availability of sufficient design and technology data. The development of the flowsheet and its integration is based on employing a systems viewpoint and systematic process synthesis techniques, amply explained over three chapters. In consequence, the solution contains elements of originality, but in each case this is compared to schemes and economic indices reported in the literature.

1.1.2
Learning by Case Studies

Practising is the best way to learn. “I see, I hear and I forget”, says an old adage, which is particularly true for passive slide-show lectures. On the contrary, “I see, I do and I understand” enables effective education and gives enjoyment.

There are two types of active learning: problem-based and project-based. The former addresses specific questions, exercises and problems, which aim to illustrate and consolidate the theory by varying data, assumptions and methods. On the contrary, the project-based learning, in which we include case studies, addresses complex and open-ended problems. These are more appropriate for solving real-life problems, for which there is no unique solution, but at least a good one, sometime “optimal”, depending on constraints and decisions. In more challenging cases a degree of uncertainty should be assumed and justified.

The principal merits of learning by case studies are that they:

1. bridge the gap between theory and practice, by challenging the students,
2. make possible better integration of knowledge from different disciplines,

3. encourage personal involvement and develop problem-solving attitude,
4. develop communication, teamwork skills and respect of schedule,
5. enable one to learn to write professional reports and making quality presentations,
6. provide fun while trying to solve difficult matters.

There are also some disadvantages that should be kept in mind, such as:

1. frustration if the workload is uneven,
2. difficulties for some students to maintain the pace,
3. complications in the case of failure of project management or leadership,
4. possibility of unfair evaluation.

The above drawbacks, merely questions of project organization, can be reduced to a minimum by taking into account the following measures:

1. provide clear definition of content, deliverables, scheduling and evaluation,
2. provide adequate support, regular evaluation of the team and of each member. If possible, separate support end evaluation, as customer/contractor relation,
3. evaluate the project by public presentation, but with individual marks,
4. propose challenging subjects issued from industry or from own research,
5. attract specialists from industry for support and evaluation.

1.1.3 Design Project

Teaching modern chemical process design can be organized at two levels:

- Teach a systems approach and systematic methods in the framework of a *process design and integration* introductory course. A period of 4–6 weeks fulltime (160 to 240 h) should be sufficient. Here, a first *process-integration project* is proposed, which can be performed individually or in small groups.
- Consolidate the engineering skills in the framework of a larger *plant design project*. A typical duration is 10–12 weeks full time with groups of 3–5 students.

Although dissimilar in extension and purpose, these projects largely share the content, as illustrated by Fig. 1.1. The main points of the approach are as follows:

1. Provide clear *definition* of the design problem. Collect sufficient engineering data. Get a comprehensive picture of chemistry and reaction conditions, thermal effects and chemical equilibrium, as well as about safety, toxicity and environmental problems. Examine the availability of physical properties for components and mixtures of significance. Identify azeotropes and key binaries. Define the key constraints.
2. The basic flowsheet structure is given by the reactor and separation systems. Alternatives can be developed by applying *process-synthesis meth*ods. Use computer simulation to get physical insights into different conceptual issues and to evaluate the performance of different alternatives.

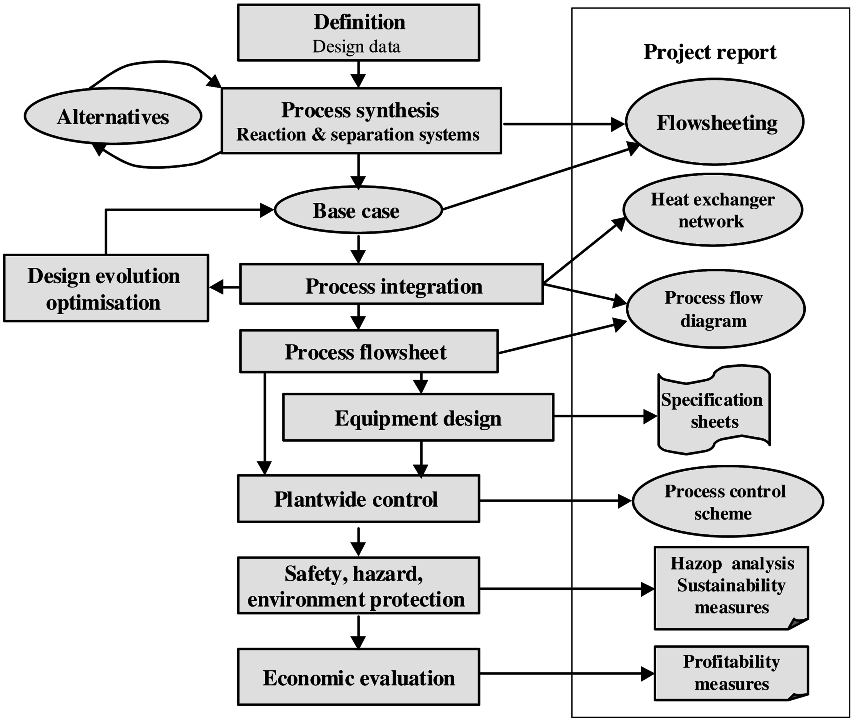

Figure 1.1 Outline of a design project.

3. Select a good base case. Determine a consistent material balance. Improve the design by using *process-integration* techniques. Determine targets for utilities, water and mass-separation agents. Set performance targets for the main equipment. Optimize the final flowsheet.

4. Perform *equipment design*. Collect the key equipment characteristics as *specification sheets*.

5. Examine *plantwide control* aspects, including safety, environment protection, flexibility with respect to production rate, and quality control.

6. Examine measures for *environment protection*. Minimize waste and emissions. Characterize process sustainability.

7. Perform the *economic evaluation*. This should be focused on profitability rather than on an accurate evaluation of costs.

8. Elaborate the *design report*. Defend it by public presentation.

In the process-integration project the goal is to encourage the students to produce original processes rather than imitate proven technologies. The emphasis is on learning a systemic methodology for flowsheet development, as well as suitable systematic methods for the design of subsystems. The emphasis is on generating flowsheet alternatives. The student should understand why several competing technologies can coexist for the same process, and be able to identify the key design decisions in each case. Thus, stimulating the creativity is the key issue at this level.

A more rigorous approach will be taught during the plant-design project. Here, the objective is to develop professional engineering skills, by completing a design project at a level of quality close to an engineering bureau. The subject may be selected from existing and proven technologies, but the rationale of the flowsheet development has to be retraced by a rigorous revision of the conceptual levels and of design decisions at each step. This time the efficiency in using materials and energy, equipment performance and the robustness of the engineering solution are central features. The quality of report and of the public presentation plays a key role in final mark. More information about this approach may be found elsewhere [1].

1.2 Sustainable Process Design

1.2.1 Sustainable Development

Sustainable development designates a production model in which fulfilling the needs of the present society preserves the rights of future generations to meet their own needs. Sustainable development is the result of an equilibrium state between economic success, social acceptance and environmental protection. Ecological sustainability demands safeguarding the natural life and aiming at zero pollution of the environment. Economic sustainability aspires to maximize the use of renewable raw materials and of green energies, and saving in this way valuable fossil resources. Social sustainability has to account of a decent life and respect of human rights in the context of the global free-market economy.

An efficient use of scarce resources by nonpolluting technologies is possible only by a large innovation effort in research, development and design. Sustainability aims at high material yield by the minimization of byproducts and waste. The same is valid for energy, for which considerable saving may be achieved by the heat integration of units and plants.

A systemic approach of the whole supply chain allows the designer to identify the critical stages where inefficient use of raw materials and energy takes place, as well as the sources of toxic materials and pollution. Developing sustainable processes implies the availability of consistent and general accepted sustainability measures. A comprehensive analysis should examine the evolution of sustainability over the whole life cycle, namely that raised by the dismantling the plant.

1.2.2 Concepts of Environmental Protection

In general, a manufacturing process can be described by the following relation [2]:

$$(A + B + I) + (M + C + H) \xrightarrow{E} P + S + R + W + F$$

The inputs – main reactants A, coreactants B and impurities I – shape the generic category of *raw materials*. In addition, *auxiliary materials* are needed for technological reasons, as reaction medium M, catalyst C, and helping chemicals H. The process requires, naturally, an amount of energy E. The outputs are: main products P, secondary products S, residues R and waste W. The term *residue* signifies all byproducts and impurities produced by reaction, including those generated from the impurities entered with the raw materials. Impurities have no selling value and are harmful to the environment. On the contrary, the secondary products may be sold. The term *waste* means materials that cannot be recycled in the process. Waste can originate from undesired reactions involving the raw materials, as well as from the degradation of the reaction medium, of the catalyst, or of other helping chemicals. The term *F* accounts for gas emissions, as CO_2, SO_2 or NO_x, produced in the process or by the generation of steam and electricity.

There are two approaches for achieving minimum waste in industry, as illustrated by Fig. 1.2 [2], briefly explained below.

1.2.2.1 Production-Integrated Environmental Protection

By this approach, the solution of the ecological problems results fundamentally from the conceptual process design. Two directions can be envisaged:

- Intrinsically protection, by eliminating at source the risk of pollution.
- Full recycling of byproducts and waste in the manufacturing process itself.

In an ecologically integrated process only saleable products should be found in outputs. Inevitably a limited amount of waste will be produced, but the overall yield of raw materials should be close to the stoichiometric requirements. By applying heat-integration techniques the energy consumption can be optimized. The economic analysis has to consider penalties incurred by greenhouse gases (GHG), as well as for the disposal of waste and toxic materials.

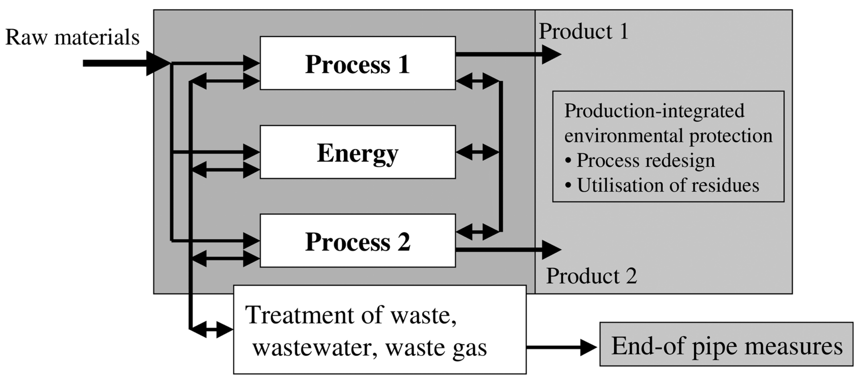

Figure 1.2 Approaches in environmental protection [2].

1.2.2.2 End-of-pipe Antipollution Measures

When a production-integrated approach cannot be applied and the amount of waste is relatively small, then end-of-pipe solutions may be employed. Examples are:

- Transformation of residues in environmental benign compounds, as by incineration or solidification.
- Cleaning of sour gases and toxic components by chemical adsorption.
- Treatment of volatile organic components (VOC) from purges.
- Wastewater treatment.

Obviously, the end-of-pipe measures can fix the problem temporarily, but not remove the cause. Sometimes the problem is shifted or masked into another one. For this reason, an end-of-pipe solution should be examined from a plantwide viewpoint and beyond. For example, sour-gas scrubbing by chemical absorption may cut air pollution locally, but involves the pollution created by the manufacture of chemicals elsewhere. In this case, physical processes or using green (recyclable) solvents are more suitable. The best way is the reduction of acid components by changing the chemistry, such as for example using a more selective catalyst.

End-of-pipe measures are implemented in the short term and need modest investment. In contrast, production-integrated environmental protection necessitates longer-term policy committed towards sustainable development.

Summing up, the following measures can be recommended for improving the environmental performances of a process:

- If possible, modify the chemical route.
- Improve the selectivity of the reaction step leading to the desired product by using a more selective catalyst. Make use primarily of heterogeneous solid catalysts, but consider pollution incurred by regeneration. If homogeneous catalysis is more efficient then developing a recycle method is necessary.
- Optimize the conversion that gives the best product distribution. Low conversion gives typically better selectivity, but implies higher recycle costs. Recycle costs can be greatly reduced by employing energy-integration and process-intensification techniques.
- Change the reaction medium that generates pollution problem. For example, replace water by organic solvents that can be recovered and recycled.
- Purify the feeds to chemical reactors to prevent the formation of secondary impurities, which are more difficult to remove.
- Replace toxic or harmful solvents and chemicals with environmentally benign materials.

1.2.3 Efficiency of Raw Materials

Measures can be used to characterize a chemical process in term of environmental efficiency of raw materials, as described below [2]. Consider the reaction:

$$\nu_A A + \nu_B B + ... \rightarrow \nu_P P + \nu_R R + \nu_S S$$

A is the reference reactant, B the coreactant, P the product, R the byproduct (valuable) and S the waste product.

Stoichiometric yield RY is defined as the ratio of the actual product to the theoretical amount that may be obtained from the reference reactant:

$$RY = \frac{\nu_A}{\nu_p} \frac{M_A}{M_P} \frac{m_p}{m_A} \tag{1.1}$$

This measure is useful, but gives only a partial image of productivity, since it ignores the contribution of other reactants and auxiliary materials, as well as the formation of secondary valuable products.

The next measures are more adequate for analyzing the efficiency of a process by material-flow analysis (MFA). Two types of materials can be distinguished:

1. Main reaction materials, which are involved in the main reaction leading to the target product. All or a part of these can be found in secondary products and byproducts in the case of more complex reaction schemes, or in residues if some are in excess and nonrecycled.
2. Secondary materials, as those needed for performing the reactions and other physical operations, as catalysts, solvents, washing water, although not participating in the stoichiometric reaction network.

The following definitions are taken from Christ [2] based on studies conducted in Germany by Steinbach (www.btc-steinbach.de).

Theoretical balance yield BA_t is given by the ratio between the moles of the target product and the total moles of the primary raw materials (PRM), including all reactants involved in the stoichiometry of the synthesis route.

$$BA_t = \frac{\text{moles target product}}{\text{moles of primary raw materials}} = \frac{n_P M_P}{\sum (n_A M_A + n_B M_B + \ldots)_{PRM}} \tag{1.2}$$

This measure considers always an ideal process, but in contrast with the stoichiometric yield, takes into account the quantitative contribution of other molecules. For this reason it is equivalent to an "atomic utilization". This parameter is constant over a synthesis route and as a result a measure of material utilization. Thus, it is the maximum productivity to be expected. A lower BA_t value means more waste in intermediate synthesis steps and a signal to improve the chemistry, by fewer intermediate steps or better selectivity.

Real balance yield BA is the ratio of the target product to the total amount of materials, including secondary raw materials (*SRM*) as solvents and catalysts, and given by:

$$BA = \frac{\text{amount target product}}{\text{amount primary and secondary materials}} = \frac{m_P}{\sum m_{PRM} + \sum m_{SRM}} \tag{1.3}$$

BA is a measure of productivity, which should be maximized by design.

The ratio of the above indices, called *specific balance yield*, is a measure of the raw material efficiency:

$$sp_{BA} = \frac{BA}{BA_t} \tag{1.4}$$

The same index can be calculated by the following relation:

$$sp_{BA} = F \times RY \times EA_p \tag{1.5}$$

The factor EA_p characterizes the efficiency of primary raw materials:

$$\begin{aligned} EA_p &= \frac{\text{amount of primary raw materials}}{\text{amount of primary and secondary raw materials}} \\ &= \frac{m_{PRM}}{\sum m_{PRM} + \sum m_{SRM}} \end{aligned} \tag{1.6}$$

The factor F expresses the excess of primary raw materials, and is defined as:

$$F = \frac{\text{stoichiometric raw materials}}{\text{excess of primary raw materials}} \leq 1 \tag{1.7}$$

From Eqs. (1.4) and (1.5) one gets:

$$BA = BA_t \times (F \times RY) \times EA_p \tag{1.8}$$

The crossexamination of the above measures can suggest means for improving the technology, in the first place the real balance yield BA. For example, the use of an excess of reactant can give higher stoichiometric yield RY, but lower real balance yield BA, if the reactant is not recycled. Hence, increasing the efficiency of primary raw materials EA_p to the theoretical limit of one is an objective of the process design. This can be achieved by replacing steps involving unrecoverable reactants and chemicals with operations where their recycle is possible. Thus, recovery and recycle of all materials inside the process is the key to sustainability from the viewpoint of material efficiency.

1.2.4 Metrics for Sustainability

The measure for assessing the sustainability of a process design should consider the complete manufacturing supply chain over the predictable plant life cycle. The metrics should be simple, understandable by a larger public, useful for decision-making agents, consistent and reproducible. The metrics described below [3] have

Example 1.1: Production of Phenone by Acetylation Reaction [2]

Phenone is produced by the acetylation of benzyl chloride with o-xylene via a Friedel–Crafts reaction. Table 1.1 presents the elements of the material balance. Calculate the efficiency of raw materials.

The stoichiometric equation is:

$$\underset{140.6}{C_6H_5\text{-}COCl} + \underset{106.2}{(C_6H_4)\text{-}(CH_3)_2} + \underset{133.4}{AlCl_3} + \underset{48}{3H_2O} =$$

$$\underset{210.2}{(C_6H_5)\text{-}CO\text{-}(C_6H_4)\text{-}(CH_3)_2} + \underset{78}{Al(OH)_3} + \underset{146}{4HCl}$$

From the relations (1.1) to (1.8) the following values result for the:

$$RY = \frac{n_P}{n_A} = \frac{4.76}{4.98} = 0.956$$

$$BA_t = \left(\frac{m_p}{\sum m_{\text{reactants}}}\right)_{\text{theoretical}} = \frac{210.2}{(140.6 + 106.2 + 133.4 + 48)} = 0.484$$

$$BA = \left(\frac{m_p}{\sum m_{\text{reactants}}}\right)_{\text{real}} = \frac{1000}{3300} = 0.303 \quad sp_{BA} = \frac{0.303}{0.484} = 0.626$$

$$EA_p = \frac{PRM}{\sum m_{\text{reactants real}}} = \frac{(700 + 550 + 700 + 258)}{3300} = 0.669$$

$$F = \frac{n_A \cdot \sum M_{\text{w,reactants}}}{\text{PRM}} = \frac{4.98(140.6 + 106.2 + 133.4 + 48)}{(700 + 550 + 700 + 258)} = 0.979$$

The calculation shows that the stoichiometric yield RY is acceptable, but the theoretical balance yield BA_t poor, because catalyst complex lost after reaction. A significant improvement would be the use of solid catalyst. Other alternative is regeneration of $AlCl_3$ complex by recycling. The two solutions would lead to the same theoretical yield, but with different costs. Therefore, a deeper investigation should take into account a cost flow analysis too. More details can be found in Christ [2].

these properties. They refer to the same unit of output, the value-added monetary unit,

$$\textit{Value-added dollar } (\$VA) = \text{Revenues} - \text{Costs of raw materials and utilities}$$

that are consistent in the sense that the lower the value the more effective the process, and indicate the same direction. A short description is given below:

Table 1.1 Material balance for the Example 1.1.

Input				Output			
	Mw	Mass	Moles		Mw	Mass	Moles
PRM				**Target product**			
R-COCl	140.6	700	4.98	Phenone	210.2	1000	4.76
o-Xylene	106.2	550	5.18				
$AlCl_3$	133.4	700	5.25	**Wastewater**			
H_2O	18	258	14.33	$Al(OH)_3$	78	410	5.26
				HCl	36.5	600	16.44
				Other		123	
SRM				**Waste**			
Toluene		900		Toluene		900	
H_2SO_4		192		Other		267	
Total		**3300**				**3300**	

PRM: primary raw materials; SRM: secondary raw materials.

1. *Material intensity* is given by the mass of waste per unit of output. Waste is calculated by subtracting the mass of products and saleable subproducts from the raw materials. Water and air are not included unless incorporated in the product.

2. *Energy intensity* is the energy consumed per unit of output. It includes natural gas, fuel, steam and electricity, all converted in net-fuel or the same unit for energy. For consistent calculations 80% average efficiency is considered for steam generation and 31% for electricity generation, corresponding to 3.138 MJ/kg steam and 11.6 MJ/kWh electricity. This metric captures in a synthetic manner the energy saving not only by heat integration, reflected by low steam and fuel consumption, but also by more advanced techniques, as cogeneration of heat and power. Negative values would mean export of energy to other processes. This situation is likely for processes involving high exothermic reactions, where the heat developed by reaction should be added as negative term in the energy balance.

3. *Water consumption* gives the amount of fresh water (excluding rainwater) per unit of output, including losses by evaporation (7% from the recycled water) and by waste treatment.

4. *Toxic emissions* consider the mass of toxic materials released per unit of output. The list of toxic chemicals can be retrieved from the website of the Environmental Protection Agency (USA).

5. *Pollutant emissions* represent the mass of pollutants per unit of output. The denominator is calculated as equivalent pollutant rather than effective mass. This topic is more difficult to quantify, but the idea is to use a unified measure.

6. *Greenhouse gas emissions* are expressed in equivalent carbon dioxide emitted per unit of output. Besides the CO_2 from direct combustion, this metric should include other sources, such as the generation of steam and electricity.

The advantage of using these measures in design is that the comparison of alternatives on a unique basis allows the designer to identify the best chemistry and flowsheet leading to the lowest resources and environmental impact. Usually the objective function is profit maximization. Including the above measures, at least as constraints, could contribute to conciliating the economic efficiency with the environmental care, a concept designated today by the label *ecoefficiency*.

A distinctive feature of these metrics is that they can be stacked along the whole product supply chain. In this way, ecological bottlenecks can be identified readily. For example, a chemical product that might appear as benign for the environment, could involve, in reality, highly toxic materials in some intermediate steps of manufacturing.

As an illustration, Table 1.2 shows values for some representative chemical processes. The output units refer to the added-value dollar $VA explained before. It can be seen that phosphoric acid has very unfavorable indices on the whole line, being very intensive as material, energy and water consumption. Acrylonitrile produced by ammonoxidation has also poor environmental performance with respect to toxics and pollutants. Note also the large amount of CO_2 produced by the methanol process. The best process in the list is the acetic acid made by the carbonylation of methanol.

Table 1.2 Sustainability metrics for some processes [3].

Process	Material kg/$	Energy MJ/$	Water m^3/$	Toxics g/$	Pollutants g/$	CO_2 kg/$
Methanol (natural gas reforming)	0.2721	165.12	0.161	5.90	0	8.80
Acetic acid (MeOH carbonylation)	0.1769	16.76	0.029	0.313	0	1.10
Terephtalic acid (p-xylene oxidation)	0.4264	47.34	0.085	35.38	2.721	3.05
Acrylonitrile (Propene ammonoxidation)	2.1228	62.74	0.121	63.50	99.789	6.22
Phosphoric acid (Wet process)	144.3	267.4	0.788	1909.62	0	17.10

Sustainability metrics can be used as decision-support instruments. Among the most important tools in *life-cycle analysis* of processes we mention:

- Practical minimum-energy requirements (PME) set reference values for the intensive-energy steps and suggests energy-reduction strategies.
- Life-cycle inventory (LCI) deals with the material inventories of each phase of a product life, namely by tracking the variation between input and output flows.

- Life-cycle assessment (LCA) consists of determining the impact on the environment of each phase of a life cycle, as material and energy intensity, emissions and toxic releases, greenhouse gases, *etc*.
- Total cost assessment (TCA) provides a comparison of costs of sustainability, and by consequence, a consistent evaluation of alternative processes.

1.3 Integrated Process Design

The principles of the systematic and systemic design of chemical-like processes have been set by the works of Jim Douglas and coworkers, largely disseminated by his book from 1988 [4]. In the field of energy saving fundamental contributions have been made by Linnhoff and coworkers [5]. Several books addressing the design by systematic methods, but from different perspectives and professional backgrounds, have been published more recently, such as by Biegler et al. [6], Seider et al. [7], Dimian [1] and Smith [8].

The assembly of the systematic methods applied to the design of chemical processes are captured today in the paradigm of *integrated process design*. The application on modern design methods becomes possible because of *process-simulation* software systems, which encode not only sophisticated computational algorithms but also a huge amount of data. Combining design and simulation allows the designer to understand the behavior of complex system and explore design alternatives, and on this basis to propose effective innovative solutions.

1.3.1 Economic Incentives

Conceptual design designates that part of the design project dealing with the basic elements defining a process: flowsheet, material and energy balances, equipment specification sheets, utility consumption, safety and environmental issues, and finally economic profitability. Therefore, in conceptual design the emphasis is on the behavior of the process as a system rather than only sizing the equipment.

It is important to note that conceptual design is responsible for the major part of the investment costs in a process plant, even if its fraction in the project's fees is rather small. An erroneous decision at the conceptual level will propagate throughout the whole chain up to the detailed sizing and procurement of equipment. Moreover, much higher costs are necessary later in the operation to correct misconceptions in the basic design. Figure 1.3 shows typical cost-reduction opportunities in a design project (Pingen [9]). It can be seen that the conceptual phase takes only a very modest part, about 2% of the total project cost, although it contributes significantly in cost-reduction opportunities, with more than 30%. In the detailed design phase the cost of engineering rises sharply to 12%, but saving opportunities goes down to only 15%. In contrast, the cost of procurement and

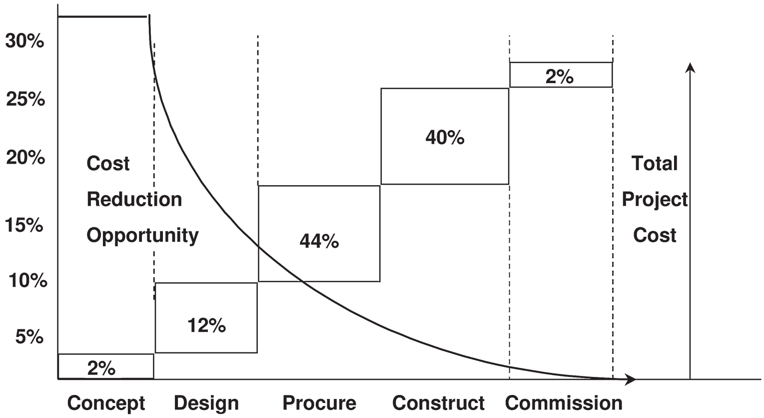

Figure 1.3 Economic incentives in a project.

construction are more than 80%, but the savings are below 10%. At the commissioning stage the total project cost is frozen.

1.3.2
Process Synthesis and Process Integration

In this book we consider the paradigm of *integrated process design* as the result of two complementary activities, process synthesis and process integration [1]. Figure 1.4 depicts the concept by means of a representation similarly with the onion diagram proposed originally by Linnhoff et al. [5]. *Process synthesis* focuses on the structural aspects that define the material-balance envelope and the flowsheet architecture. The result is the solution of the layers regarding the reaction (R) and the separation (S) systems, including the recycles of reactants and mass-separation agents. *Process integration* deals mainly with the optimal use of heat (H) and utilities (U), but includes two supplementary layers for environmental protection (E), as well as for controllability, safety and operability (C).

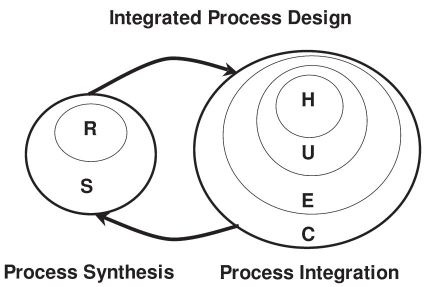

Figure 1.4 Integrated process design approach.

The key features of an integrated process design are:

1. The main objective of design is the *flowsheet architecture*. We mean by this type of units, performance and connections by material and energy streams. Systemic techniques are capable of calculating optimal targets for subsystems and components without the need of the detailed sizing of equipment.
2. The approach consists of developing alternatives rather than a unique flowsheet. The selected solution is the best cost-effective means only for the assumed constraints of technological, ecological, economical and social nature.
3. Computer simulation is the key tool for analysis, synthesis and evaluation of designs. The efficiency in using the software depends on the capacity of the designer to integrate generic capabilities with particular engineering knowledge.
4. The methodology addresses new design, debottlenecking and retrofit projects, and it can be applied to any type of process industries.

We stress again the importance of developing alternatives in which design targets are set well ahead of the detailed sizing of equipment. The last feature indicates a qualitative change that is removed from the concept of unit operations in favor of a more generic approach based on generic *tasks*. Using tasks instead of standard unit operations facilitates the invention of nonconventional equipment that can combine several functionalities, such as reaction and separations. This approach is designated today by *process intensification*. Moreover, the task-oriented design is more suited for applying modern process-synthesis techniques based on the optimization of superstructures.

1.3.3 Systematic Methods

The long road from an idea to a real process can be managed at best by means of a systemic approach. A design methodology consists of a combination of analysis and synthesis steps. *Analysis* is devoted to the knowledge of the elements of a system, such as for example the investigation of physical properties of species and mixtures, the study of elements characterizing the performance of reactors and unit operations, or the evaluation of profitability. *Synthesis* deals with activities aiming to determine the architecture of the system, as the selection of suitable components, their organization in the frame of a structure, as well as with the study of connections and interactions.

A design problem is always *underdefined*, either by the lack of data or insufficient time and resources. Moreover, a design problem is always *open-ended* since the solution depends largely on the *design decisions* taken by the designer at different stages of project development, for example to fulfil technical or economical constraints, or to avoid a license problem.

The systematic *generation of alternatives* is the most important feature of the modern conceptual design. The best solution is identified as the optimal one in the context of constraints by using consistent evaluation and ranking of alternatives. In the last two decades, a number of powerful systematic techniques have emerged to support the integrated process design activities. These can be classified roughly as:

- heuristics-based methods,
- thermodynamic analysis methods,
- optimization methods.

Note that so-called heuristics does not mean necessarily empirical-based rules. Most heuristics are the results of fundamental studies or extensive computer simulation, but may be formulated rather as simple decisional rules than by means of mathematical algorithms.

Today, the field of integrated process design is an active area of scientific research with immediate impact on the engineering practice. Methods accepted by the process-engineering community are described briefly below.

1.3.3.1 Hierarchical Approach

The hierarchical approach is a generic methodology for laying out the conceptual flowsheet of a process. The methodology consists of decomposing a complex problem into simpler subproblems. The approach is organized in "levels" of design decisions and flowsheet refinement. Each level makes use of heuristics to generate alternatives. Consistent evaluation eliminates unfeasible alternatives, keeping only a limited number of schemes for further development. Finally, the methodology allows the designer to develop a good "base case", which can be further refined and optimized by applying process-integration techniques. Chapters 2 to 4 present a revisited approach with respect to a previous presentation [1].

1.3.3.2 Pinch-Point Analysis

Pinch-point analysis deals primarily with the optimal management of energy, as well as with the design of the corresponding heat-exchanger network. The approach is based on the identification of the *pinch point* as the region where the heat exchange between the process streams is the most critical. The pinch concept has been extended to other systemic issues, as process water saving and hydrogen management in refineries. More details about this subject can be found in the monograph by Linnhoff et al. [5], as well as in the recent book by Smith [8].

1.3.3.3 Residue Curve Maps

The feasibility of separations of nonideal mixtures, as well as the screening of mass-separation agents for breaking azeotropes can be rationalized by means of thermodynamic methods based on residue curve maps. The treatment was extended processes with simultaneous chemical reaction. Two comprehensive books have been published recently by Stichlmair and Frey [10], as well as by Doherty and Malone [11].

1.3.3.4 **Superstructure Optimization**

A process-synthesis problem can be formulated as a combination of tasks whose goal is the optimization of an economic objective function subject to constraints. Two types of mathematical techniques are the most used: mixed-integer linear programming (MILP), and mixed-integer nonlinear programming (MINLP).

Process synthesis by superstructure optimization consists of the identification of the best flowsheet from a superstructure that considers many possible alternatives, including the optimal one. A substantial advantage is that integration and design features may be considered simultaneously. At today's level of software technology the superstructure optimization is still an emerging technique. However, notable success has been achieved in numerous applications. The reference in this field is the book of Biegler et al. [6].

1.3.3.5 **Controllability Analysis**

Plantwide control can be viewed as the strategy of fulfilling the production objectives of a plant, such as keeping optimal the material and energy balance, while preserving safety and waste minimization. Plantwide control means also that the global control strategy of the plant has to be compatible with the local control of units, for which industry proven solutions exist. Controllability analysis consists of evaluating the capacity of a process to be controlled. The power of manipulated variables should be sufficient (this is a design problem) to effectively keep the controlled variables on setpoints for predictable disturbances, or to move the plant onto new setpoints when changing the operation procedure. Controllability analysis and plantwide control can be handled today by a systematic approach. For a deeper study see the books of Luyben and Tyreus [12], Skogestad and Postlewaite [13], Dimian [1], as well as the recent monograph edited by Seferlis and Georgiadis [14].

1.3.4
Life Cycle of a Design Project

Life-cycle models can be used to manage the elaboration of complex projects [1]. A simple but efficient model can be built up on the basis of a waterfall approach. This indicates that the project sequencing should be organized so as to avoid excessive feedback between phases, and in particular to upset the architectural design. More sophisticated approaches, such as V-cycle or spiral models, could be used to handle projects requiring more flexibility and uncertainty, as in the case of software technology.

As a general approach by systems engineering, the phases of a project must be clearly defined such as the output of one stage falls cleanly into the input of the next stage. Complete definition of goals and requirements comes first. Systemic (architectural) design always precedes the detailed design of components. The modeling of units should be at the level of detail capable of capturing the behavior of the system, not more. After solving appropriately the conceptual phase, the

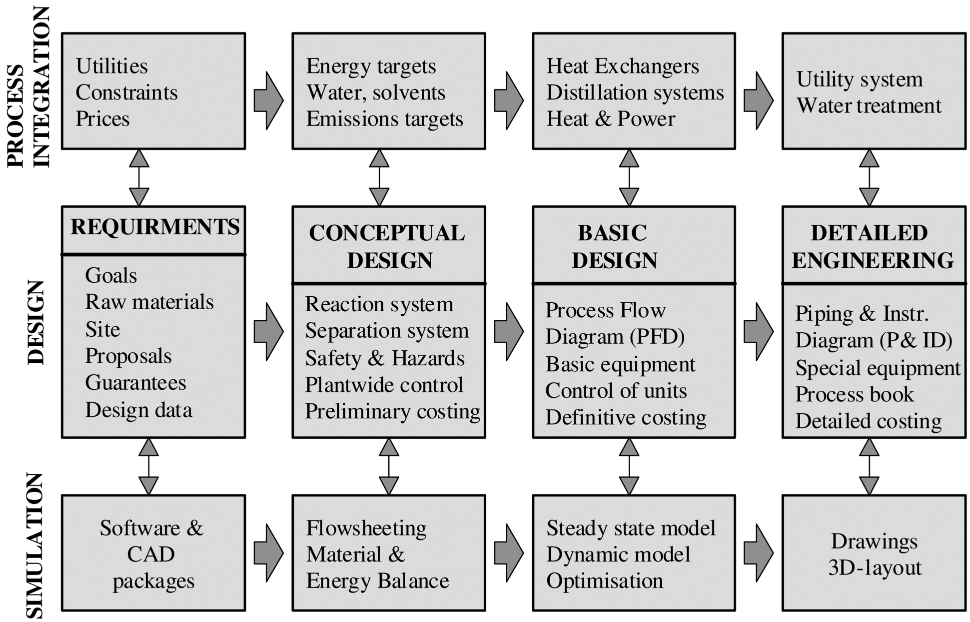

Figure 1.5 Life cycle of an integrated design project [1].

project may proceed with the implementation and test of units, and finally with the test of the system, in most cases by computer simulation.

The development of an idealized process design project can be decomposed into four major phases: *requirements, conceptual design, basic design*, and *detailed engineering*, as shown in Fig. 1.5. Typical integration and simulation activities are listed. For example, the flowsheet developed during the conceptual design consists mainly of the reaction and separation subsystems. Other issues solved at this level are safety and hazards, environmental targets, plantwide control objectives and preliminary economic evaluation. By process-integration techniques targets for utilities, water and solvents are assessed. Several alternatives are developed, but only one base case is selected for further refinement. In this phase, process simulation is a key activity for getting consistent material and energy balances.

The development of the selected alternative is continued in the *basic design* phase, by the integration of subsystems, which leads to final process flow diagram (PFD). Specific integration activities regard the design of the heat-exchanger network, the energy saving in distillations, or combined heat and power generation.

Completing the flowsheet allows the generation of a steady-state simulation model. A dynamic simulation model may be developed for supporting process control implementation and for the assessment of operation strategies.

In *detailed engineering*, the components of the project are assembled before commissioning.

In practice, the workflow of a project may be different from the idealized frame presented above. For example, parallel engineering may be used to improve the overall efficiency. However, recognizing the priority of conceptual tasks and minimizing the structural revisions remain key factors.

1.4 Summary

Innovation is the key issue in today's chemical process industries. The main directions are *sustainability* and *process intensification*. Sustainability means in the first place the efficient use of raw materials and energy close to the theoretical yields. By process intensification the size of process plants is considerably reduced. The integration of several tasks in the same unit, as in reactive separations, can considerably simplify the flowsheet and decrease both capital and operation costs.

Production-integrated environmental protection implies that ecological issues are included in the conceptual design at very early stages. This approach should prevail over the end-of-pipe measures, which shift but do not solve the problem.

Increasing recycling of materials and energy results in highly integrated processes. Saving resources and preserving flexibility in operation could raise conflicts. These can be prevented by integrating flowsheet design and plantwide control.

By a systems approach, a process is designed as a complex system of interconnected components so as to satisfy agreed-upon measures of performance, such as high economic efficiency of raw materials and energy, down to zero waste and emissions, together with flexibility and controllability faced with variable production rate.

Integrated process design is the paradigm for designing efficient and sustainable processes. Key features are:

- Integrated flowsheet architecture for a cost-effective process is the main objective. Appropriate systemic techniques are capable of determining close-to-optimum targets for components without the need for detailed design and sizing.
- The conceptual design consists of developing several alternatives rather than a single flowsheet. The reason for alternatives is that every development step is controlled by design decisions. The selected solution among the alternatives should fulfil at best the optimization criteria within the environment of constraints.
- Process simulation is the main conceptual tool, both for analysis and synthesis purposes. Today, the traditional art-of-engineering is replaced by accurate computer simulation. Modern steady-state and dynamic simulation techniques make possible the investigation of complex processes close to the real situation.

- Getting accurate data, namely for thermodynamic and kinetic modeling, remains a challenge. For this reason, confronting the predictions by simulation with industrial reality is necessary, each time when this is possible.
- The systematic methods and the analysis tools of integrated process design can be applied to any type of chemical process industries, from refining to biotechnologies, as well as to new or revamped projects.
- For assessing the sustainability of process design consistent measures should be applied, such to minimize the material waste, energy, water consumption, toxic and pollutant emissions per unit of added value.
- The management of design project can be ensured by adopting the life-cycle modeling approach, in which the key elements are recognizing the priority of conceptual tasks and minimizing the structural revisions.

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