1
Why Modelling?

Analysis of the cognition methods which have been used since early times reveals that the general methods created in order to investigate life phenomena could be divided into two groups: (i) the application of similitude, modelling and simulation, (ii) experimental research which also uses physical models. These methods have always been applied to all branches of human activity all around the world and consequently belong to the universal patrimony of human knowledge. The two short stories told below aim to explain the fundamental characteristics of these cognition methods.

First story. When, by chance, men were confronted by natural fire, its heat may have strongly affected them. As a result of these ancient repeated encounters on cold days, men began to feel the agreeable effect of fire and then wondered how they could proceed to carry this fire into their cold caves where they spent their nights. The precise answer to this question is not known, but it is true that fire has been taken into men's houses. Nevertheless, it is clear that men tried to elaborate a scheme to transport this natural fire from outside into their caves. We therefore realize that during the old times men began to exercise their minds in order to plan a specific action. This cognition process can be considered as one of the oldest examples of the use of modelling research on life.

So we can hold in mind that the use of modelling research on life is a method used to analyze a phenomenon based on qualitative and quantitative cognition where only mental exercises are used.

Second Story. The invention of the bow resulted in a new lifestyle because it led to an increase in men's hunting capacity. After using the bow for the first time, men began to wonder how they could make it stronger and more efficient. Such improvements were repeated continually until the effect of these changes began to be analysed. This example of human progress illustrates a cognition process based on experimentation in which a physical model (the bow) was used.

In accordance with the example described above, we can deduce that research based on a physical model results from linking the causes and effects that characterize an investigated phenomenon. With reference to the relationships existing between different investigation methods, we can conclude that, before modifying

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the physical model used, modelling research has to be carried out. The modelling can then suggest various strategies but a single one has to be chosen. At the same time, the physical model used determines the conditions required to measure the effect of the adopted strategy. Further improvement of the physical model may also imply additional investigation.

If we investigate the scientific and technical evolution for a random selected domain, we can see that research by modelling or experimentation is fundamental. The evolution of research by modelling and/or experimentation (i.e. based on a physical model) has known an important particularization in each basic domain of science and techniques. Research by modelling, by simulation and similitude as well as experimental research, have become fundamental methods in each basic scientific domain (such as, in this book, chemical engineering). However, they tend to be considered as interdisciplinary activities. In the case of modelling simulation and similitude in chemical engineering, the interdisciplinary state is shown by coupling the phenomena studied with mathematics and computing science.

1.1
Process and Process Modelling

In chemical engineering, as well as in other scientific and technical domains, where one or more materials are physically or chemically transformed, a process is represented in its abstract form as in Fig. 1.1(a). The global process could be characterized by considering the inputs and outputs. As input variables (also called "independent process variables", "process command variables", "process factors" or "simple factors"), we have deterministic and random components. From a physical viewpoint, these variables concern materials, energy and state parameters, and of these, the most commonly used are pressure and temperature. The deterministic process input variables, contain all the process variables that strongly influence the process exits and that can be measured and controlled so as to obtain a designed process output.

The random process input variables represent those variables that influence the process evolution, but they can hardly be influenced by any external action. Frequently, the random input variables are associated with deterministic input variables when the latter are considered to be in fact normal randomly distributed variables with mean $\bar{x}_j,\ j = 1, N$ ("mean" expresses the deterministic behaviour of variable x_j) and variance $\sigma_{xj},\ j = 1, N$. So the probability distribution function of the x_j variable can be expressed by the following equation:

$$f(x_j) = \frac{1}{\sqrt{2\pi}\sigma_{xj}} \exp\left(-\frac{(x_j - \bar{x}_j)^2}{2\sigma_{xj}^2}\right) \qquad (1.1)$$

The values of $\bar{x}_j,\ j = 1, N$ and $\sigma_{xj},\ j = 1, N$ can be obtained by the observation of each x_j when the investigated process presents a steady state evolution.

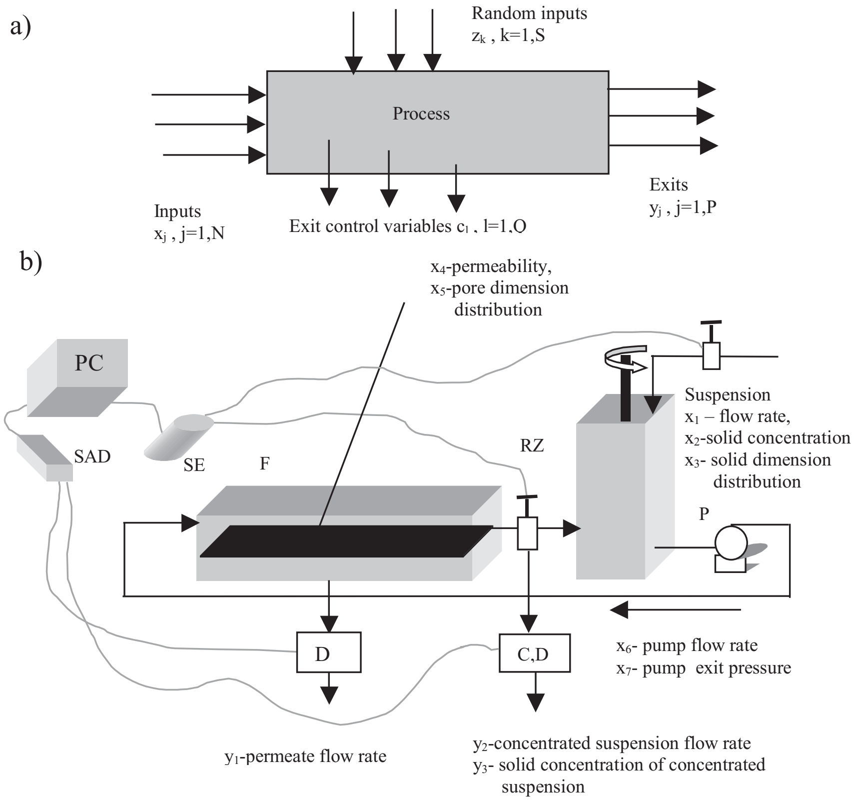

Figure 1.1 The abstract (a) and concrete (b) drawing of a tangential filtration unit.

The exit variables that present an indirect relation with the particularities of the process evolution, denoted here by $c_l, l = 1, Q$, are recognized as intermediary variables or as exit control variables. The exit process variables that depend strongly on the values of the independent process variables are recognized as dependent process variables or as process responses. These are denoted by $y_i, i = 1, P$. When we have random inputs in a process, each y_i exit presents a distribution around a characteristic mean value, which is primordially determined by the state of all independent process variables $\bar{x}_j$, $j = 1, N$. Figure 1.1 (b), shows an abstract scheme of a tangential filtration unit as well as an actual or concrete picture.

Here F filters a suspension and produces a clear filtrate as well as a concentrated suspension which is pumped into and out of reservoir RZ. During the process a fraction of the concentrated suspension is eliminated. In order to have a continuous process it is advisable to have working state values close to steady state values. The exit or output control variables (D and CD registered) are connected to a data acquisition system (DAS), which gives the computer (PC) the values of the filtrate flow rate and of the solid concentration for the suspension transported.

The decisions made by the computer concerning the pressure of the pump-flow rate dependence and of the flow rate of the fresh suspension, are controlled by the micro-device of the execution system (ES). It is important to observe that the majority of the input process variables are not easily and directly observable. As a consequence, a good technological knowledge is needed for this purpose. If we look attentively at the $x_1 - x_5$ input process variables, we can see that their values present a random deviation from the mean values. Other variables such as pump exit pressure and flow rate (x_6, x_7) can be changed with time in accordance with technological considerations.

Now we are going to introduce an automatic operation controlled by a computer, which means that we already know the entire process. Indeed, the values of y_1 and y_3 have been measured and the computer must be programmed with a mathematical model of the process or an experimental table of data showing the links between dependent and independent process variables. Considering each of the unit devices, we can see that each device is individually characterised by inputs, outputs and by major phenomena, such as the flow and filtration in the filter unit, the mixing in the suspension reservoir and the transport and flow through the pump. Consequently, as part of the unit, each device has its own mathematical model. The global model of the plant is then the result of an assembly of models of different devices in accordance with the technological description.

In spite of the description above, in this example we have given no data related to the dimensions or to the performance of the equipment. The physical properties of all the materials used have not been given either. These data are recognized by the theory of process modelling or of experimental process investigation as process parameters. A parameter is defined by the fact that it cannot determine the phenomena that characterize the evolution in a considered entity, but it can influence the intensity of the phenomena [1.1, 1.2].

As regards the parameters defined above, we have two possibilities of treatment: first the parameters are associated with the list of independent process variables: we will then consequently use a global mathematical model for the unit by means of the formal expression (1.2). Secondly, the parameters can be considered as particular variables that influence the process and then they must, consequently, be included individually in the mathematical model of each device of the unit. The formal expression (1.3) introduces this second mathematical model case:

$$y_i = F(x_1, x_2 ....., x_N, z_1, z_2 ....., z_S) \qquad i = 1, ...P \tag{1.2}$$

$$y_i = F(x_1, x_2 ....., x_N, z_1, z_2 ....., z_S, p_1, p_2, ..., p_r) \qquad i = 1, ...P \tag{1.3}$$

We can observe that the equipment is characterized by the process parameters of first order whereas process parameters of second order characterize the processed materials. The first order and second order parameters are respectively called “process parameters” and “non-process parameters”.

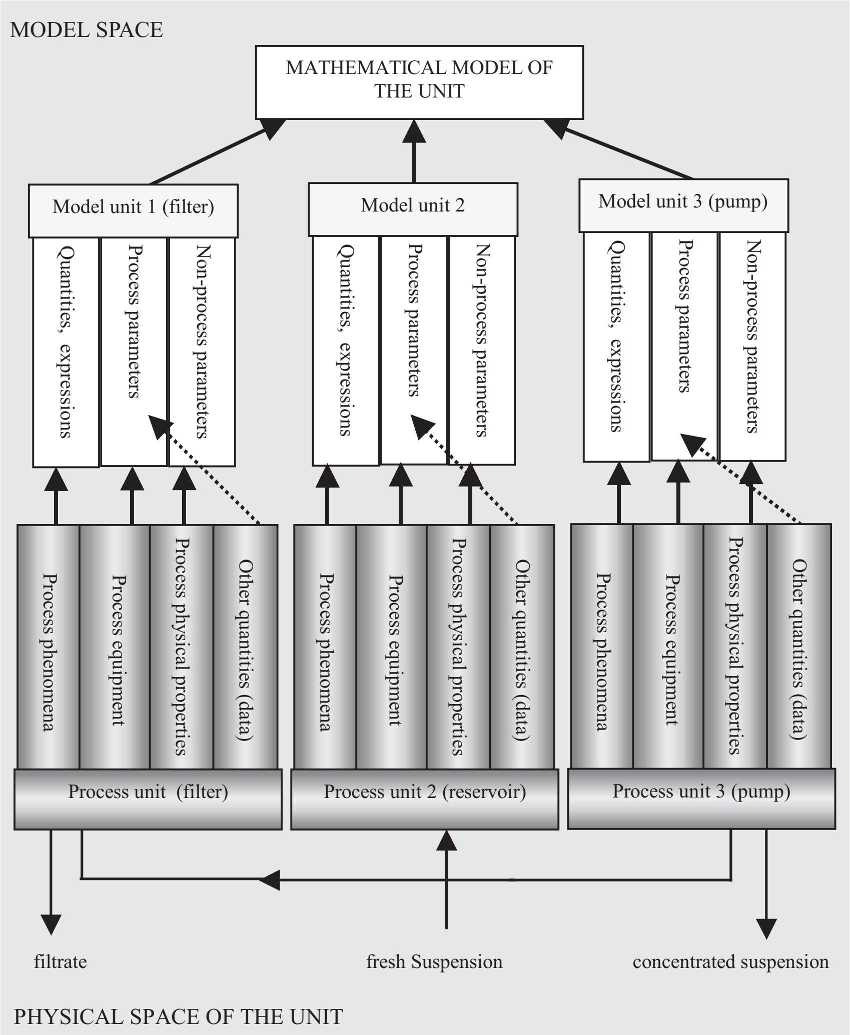

Figure 1.2 Process and model parts (extension of the case shown in Fig. 1.1(b)).

Figure 1.2 shows a scheme of the physical space of the filtration unit and of its associated model space. The model space presents a basic level which includes the model of each device (filter, reservoir and pump) and the global model which results from the assembly of the different models of the devices.

If we establish a relation between Fig. 1.2 and the computer software that assists the operation of the filtration plant, then we can say that this software can be the result of an assembly of mathematical models of different components or/ and an assembly of experimentally characterized components.

It is important to note that the process control could be described by a simple or very complex assembly of relations of type (1.2) or (1.3). When a model of one component is experimentally characterized in an assembly, it is important to correct the experimental relationships for scaling-up because these are generally obtained by using small laboratory research devices. This problem can be solved by dimensional analysis and similitude theory. From Fig. 1.2 we can deduce that the first step for process modelling is represented by the splitting up of the process into different elementary units (such as component devices, see Fig. (1.1b)). As far as one global process is concerned, each phenomenon is characterized by its own model and each unit (part) by the model of an assembly of phenomena.

A model is a representation or a description of the physical phenomenon to be modelled. The physical model (empirical by laboratory experiments) or conceptual model (assembly of theoretical mathematical equations) can be used to describe the physical phenomenon. Here the word “model” refers to a mathematical model. A (mathematical) model as a representation or as a description of a phenomenon (in the physical space) is a systematic collection of empirical and theoretical equations. In a model (at least in a good model) both approaches explain and predict the phenomenon. The phenomena can be predicted either mechanistically (theoretically) or statistically (empirically).

A process model is a mathematical representation of an existing or proposed industrial (physical or/and chemical) process. Process models normally include descriptions of mass, energy and fluid flow, governed by known physical laws and principles. In process engineering, the focus is on processes and on the phenomena of the processes and thus we can affirm that a process model is a representation of a process. The relation of a process model and its structure to the physical process and its structure can be given as is shown in Fig. 1.2 [1.1–1.3].

A plant model is a complex mathematical relationship between the dependent and independent variables of the process in a real unit. These are obtained by the assembly of one or more process models.

1.2
Observations on Some General Aspects of Modelling Methodology

The first objective of modelling is to develop a software that can be used for the investigation of the problem. In this context, it is important to have more data about the modelling methodology. Such a methodology includes: (i) the splitting up of the models and the definition of the elementary modelling steps (which will then be combined to form a consistent expression of the chemical process); (ii) the existence of a generic modelling procedure which can derive the models from scratch or/and re-use existing models by modifying them in order to meet the requirements of a new context.

If we consider a model as a creation that shows the modelled technical device itself, the modelling process, can be considered as a kind of design activity [1.4, 1.5]. Consequently the concepts that characterize the design theory or those related to solving the problems of general systems [1.6, 1.7] represent a useful starting base for the evolution of the modelling methodology. Modelling can be used to create a unit in which one or more operations are carried out, or to analyse an existing plant. In some cases we, a priori, accept a split into different components or parts. Considering one component, we begin the modelling methodology with its descriptive model (this will also be described in Chapter 3). This descriptive model is in fact a splitting up procedure, which thoroughly studies the basic phenomena. Figure 1.3 gives an example of this procedure in the case of a liquid–solid extraction of oil from vegetable seeds by a percolation process. In the descriptive model of the extraction unit, we introduce entities which are endowed with their own attributes. Considering the seeds which are placed in the packed bed through which the extraction solvent is flushed, we introduce the "packed bed and mono-phase flow" entity. It is characterized by different attributes such as: (i) dynamic and static liquid hold-up, (ii) flow permeability and (iii) flow dispersion. The descriptive model can be completed by assuming that the oil from the seeds is transported and transferred to the flowing solvent. This assumption introduces two more entities: (i) the oil seed transport, which can be characterized by one of the following attributes: core model transport or porous integral diffusion model transport, and (ii) the liquid flow over a body, that can be characterized by other various attributes. It is important to observe that the attributes associated to an entity are the basis for formulation of the equations, which express the evolution or model of the entity.

The splitting up of the process to be modelled and its associated mathematical parts are not unique and the limitation is only given by the researcher's knowledge. For example, in Fig. 1.3, we can thoroughly analyse the splitting up of the porous seeds by introducing the model of a porous network and/or a simpler porous model. Otherwise we have the possibility to simplify the seed model (core diffusion model or pure diffusion model) into a model of the transport controlled by the external diffusion of the species (oil). It is important to remember that sometimes we can have a case when the researcher does not give any limit to the number of splits. This happens when we cannot extend the splitting because we do not have any coherent mathematical expressions for the associated attributes. The molecular scale movement is a good example of this assertion. In fact we cannot model this type of complex process by using the classical transport phenomena equations. Related to this aspect, we can say that the development of complex models for this type of process is one of the major objectives of chemical engineering research (see Section 1.4).

Concerning the general aspects of the modelling procedure, the definition of the modelling objectives seems largely to be determined by the researcher's pragmatism and experience. However, it seems to be useful in the development and the resulting practical use of the model in accordance with the general principles of scientific ontology [1.8, 1.9] and the general system theory [1.10]. If a model is developed by using the system theory principles, then we can observe its structure and behaviour as well as its capacity to describe an experiment such as a real experimental model.

Concerning the entities defined above (each entity together with its attributes) we introduce here the notion of basic devices with various types of connections.

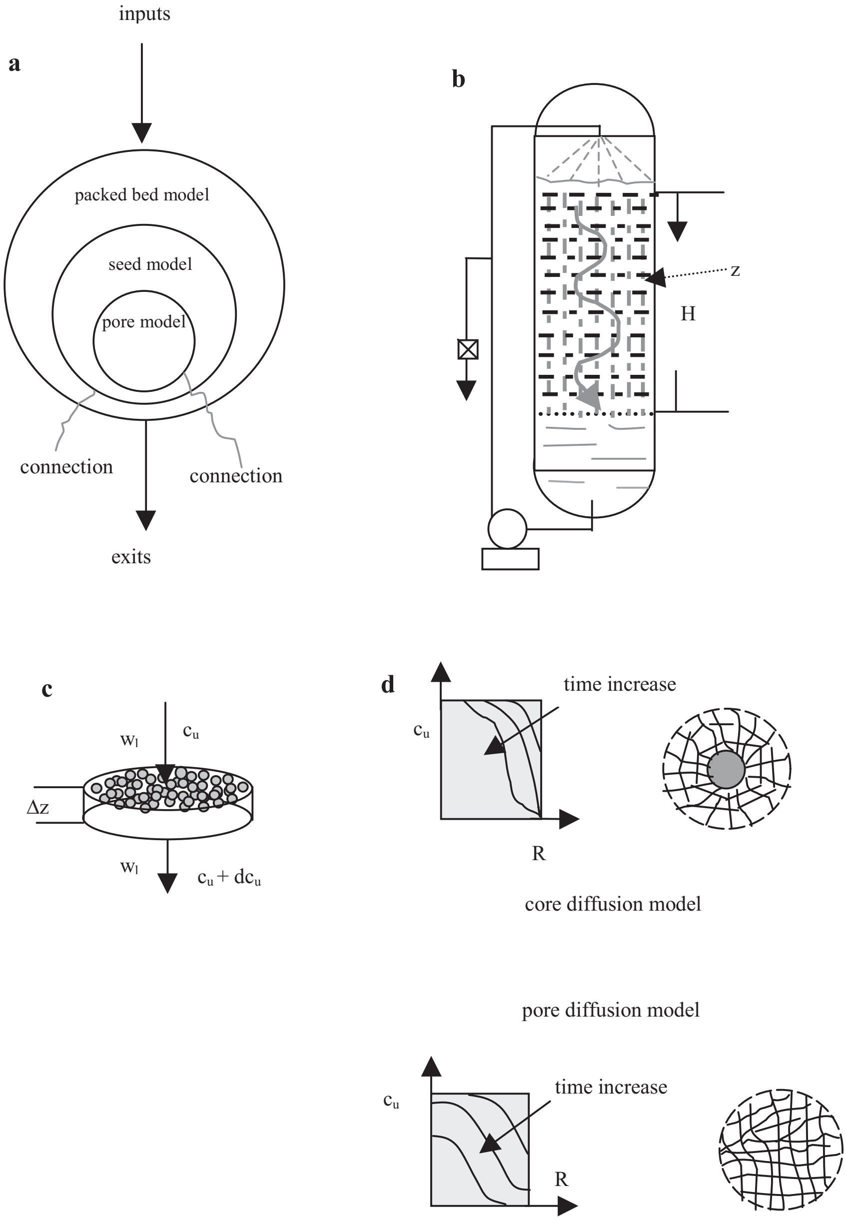

Figure 1.3 Entities and attributes for percolation extraction of oil from seeds.
(a) Hierarchy and connections of the model,
(b) percolation plant,
(c) section of elementary length in packed seeds bed,
(d) physical description of two models for oil seed transport

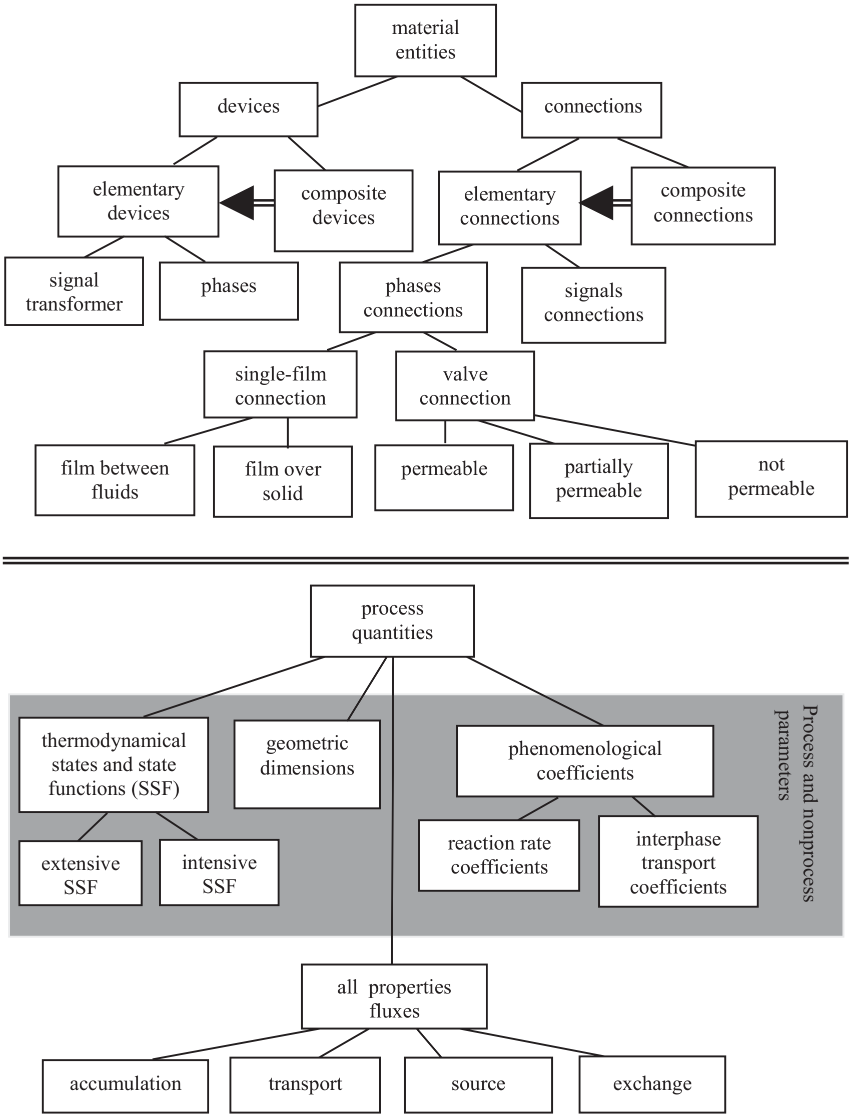

Figure 1.4 Material entities and process quantities for the development of a structured mathematical modelling.

One of the characteristics of basic devices is that they cannot be split up into parts. A basic device can also be a signal transformer (a function which transforms the input into output, such as the thermocouple that transforms the input temperature into an electrical tension). The process phases are connected and characterized quantitatively, from the viewpoint of characteristic relations (equations), as in Fig. 1.4 [1.11–1.13]. This structured mathematical modelling development corresponds to the case of a modelling based on transport phenomena, which are analysed in Chapter 3. Now, we shall give some explanation concerning some aspects of the basic chemical engineering introduced in Fig. 1.4. With respect to the generalized fluxes and their refinements, it is known that they directly correspond to the physicochemical phenomena occurring in a phase or at its boundary according to the phase properties. Otherwise, any process quantity assigned to a particular phase may depend on one or several coordinates such as time and spatial dimensions.

Various laws restrict the values of the process quantities. These laws may represent either fundamental, empirical physicochemical relationships or experimentally identified equations (from statistical modelling or from dimensional analysis particularizations). In contrast to statistical or dimensional analysis based models [1.14], which are used to fix the behaviour of signal transformers, the models of transport phenomena are used to represent generalized phases and elementary phase connections. Here, the model equations reveal all the characterizing attributes given in the description of a structure. They include *balance equations, constitutive equations* and *constraints.*

The last introduced notions show that the modelling methodology tends to a scientific synthetic working procedure, where the use of an abstract language is needed to unify the very high diversity of cases that require an analysis made by mathematical modelling. At the same time the problem discussed here has shown that the creation of models could be considered as a special problem of design and modelling, i.e.could be considered as an art rather than a science [1.15], emphasizing a modeller's creativity and intuition rather than a scientific methodology.

1.3
The Life-cycle of a Process and Modelling

The life-cycle of a chemical compound production or of a chemical process development starts when a new and original idea is advanced taking into account its practical implementation. The former concept with respect to the process life-cycle, which imposed a rigid development from research and development to process operation, has been renewed [1.16–1.18]. It is well known that the most important stages of the life-cycle of a process are research and development, conceptual design, detailed engineering, piloting and operation. These different steps partially overlap and there is some feedback between them as shown in Fig. 1.5. For example, plant operation models can be the origin of valuable tips and potential research topics, obviously these topics directly concern the research and development steps (R&D). The same models, with some changes, are preferably utilized in all the steps. The good transfer of information, knowledge and ideas is important for successfully completion of the development of all the process phases. For this purpose, it is important to have a proper documentation of underlying theories and assumptions about the model (models). This acts as a check list when a problem occurs and ensures that knowledge is transferred to the people concerned. The models are an explicit way of describing the knowledge of the process and related phenomena. They provide a systematic approach to the problems in all the stages of the process life-cycle. In addition, the process of writing the theory as mathematical expressions and codes, reveals the deficiencies with respect to the form and content.

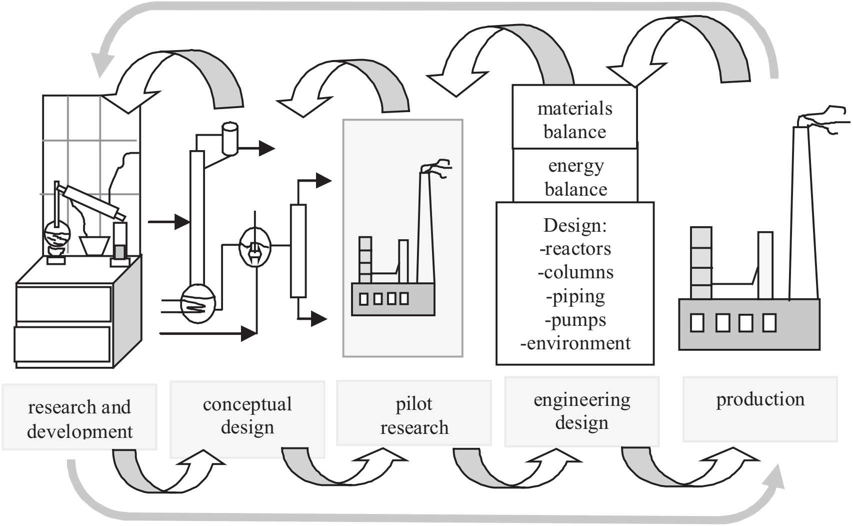

Figure 1.5 The stages of the process life-cycle and their main relationships.

Among the factors that influence the amount of work required to develop a model, we can retain the complexity, the novelty and the particular knowledge related to the process in modelling. Otherwise, commercial modelling software packages are frequently used as an excellent platform. In the following sections we detail some particularities of the models used in the process life-cycle.

1.3.1
Modelling and Research and Development Stage

The models in the R&D stage can first be simple, and then become more detailed as work proceeds. At this stage, attention has to be focused on the phenomena of phase equilibrium, on the physical properties of the materials, on chemical kinetics as well as on the kinetics of mass and heat transfer. As previously shown (see Figs 1.2 and 1.3), the decomposition of the process into different elementary units is one of the first activities. This action requires careful attention especially because, at this life-cycle stage, the process could be nothing but an idea. The work starts with the physical properties, as they act as an input to all other components. The guidelines to choose physical properties, phase equilibrium data, characteristic state equations etc. can be found in the usual literature. For each studied case, we can choose the level of detail such as the complexity of the equations and the number of parameters. If the literature information on the physical properties is restricted an additional experimental step could be necessary. As far as industrial applications are concerned, the estimation of the reaction kinetics is usually semi-empirical. Therefore, a full and detailed form of kinetics equations is not expected for the majority of the investigated cases. Some physical phenomena along with their effects can require special attention. Conventional engineering correlations may not apply, and, consequently, the research must be directed to study of these problems.

The ideal modelling and experimental work have to be realized simultaneously and are strongly related. Models provide a basis to choose, both qualitatively and quantitatively, appropriate experimental conditions. The data obtained from experimental work are used to confirm or reject the theories or the form of equations if an empirical model is being applied. Otherwise, these data are used to estimate the model parameters. This work is sequential in the sense that starting from an initial guess, the knowledge of the system grows and models get more and more accurate and detailed as the work proceeds. With a proper experimental design, the models can be used to evaluate and to rank competitive theories. Since, at the research and development (R&D) stage, models are still in the building phase, they can mainly be used for experimental design.

When the R&D steps are almost completed, the models related to the phenomena are combined into process unit models. Bench scale tests are used to check separate process ideas. The estimation of the equipment parameters can be seen as R&D work, especially if the equipment is in some way new, such as a new innovation or a new application. Based on a good knowledge of the phenomena, valuable tips concerning optimal operating parameters (such as temperature and pressure range as well as restricting phenomena) can be given to the next stages. In this stage we can meet several important sub-problems to select the appropriate models. There are often competitive theories to describe the relevant phenomena. A choice has also to be made between mechanistic and empirical approaches. The former should be favoured but an integrated solution is usually more beneficial. Then, the degree of detail has to be chosen in order to serve the model usefully. Practically, the best solution is to describe the most relevant phenomena in a detailed way, whereas the less important ones will be left approximate or in an empirical state.

1.3.2
Modelling and Conceptual Design Stage

The establishing of the optimal process structure and the best operating conditions characterizes the process development at this stage. Firstly, attention must be focused on the synthesis of the proceess. The extent to which models can be used in this phase varies. If we have a new process, information from similar cases may not be available at this stage. In the opposite situation, when the chemical components are well known, which usually means that their properties and all related parameters can be found in databanks, the models can be used to quickly check new process ideas. For example, at this stage, for a multiple-component distillation problem, models are used to identify key and non-key components, optimum distillation sequence, the number of ideal stages, the position of feed, etc. At this stage also, we always focus on the full-scale plant. Another question is how the concept will be carried out in the pilot phase. It is known that for this (piloting) stage, the equipment does not have to be a miniature of the full scale. Practice has shown that the choices made here affect both investment and operating costs later on. An image of the full-scale plant should also be obtained. The researchers who work at this level will propose some design computations which are needed by the piloting stage of process life-cycle. Their flow-sheet is the basis of the pilot design or development.

1.3.3
Modelling and Pilot Stage

The whole process concept is generally improved in the pilot plant. We can transform this stage into a process analysis made of models if enough experimental data and knowledge about the process exist (for example when we reuse some old processes). For reference, we should mention that other situations are important, such as, for example, knowing that a pilot plant provides relatively easy access to the actual conditions of the process. Some by-pass or small streams could be taken off from the pilot unit and be used in the operation of apparatuses specially designed for the experimental work. Now the models should be ready, except for the correct values of the parameters related to the equipment. A special pilot stage feature consists in adding the equations describing the non-ideal process hardware to the model in order to compute efficiency (tray efficiency, heat exchanger efficiency, non-ideality numbers, etc). This stage is strongly limited in time, so, to be efficient, researchers must prepare a careful experimental program. It may be impossible to foresee all the details, since the experimentation related to the estimation of parameters is often carried out in sequences, but still, a systematic preparation and organization of the work to be done remains useful. Since a pilot plant is rigid as far as its manœuvrability is concerned, full advantage should be taken of all the data acquired with its help. Data loggers are recommended to collect and store process data and also to provide customized data reports for modelling. If we link the process data logger with the laboratory information system, then there is a good possibility of getting a full image of the state of the process at a precise time. It is important to remember, that the goal of the pilot stage in terms of modelling is to get a valid mass and energy balance model and to validate the home-made models.

1.3.4
Modelling and Detailed Engineering Stage

In this stage, models are used for the purpose for which they have been created: the design and development of a full scale plant which is described in the detailed engineering stage. On the basis of what has been learned before, the equipment can be scaled-up, taking into consideration pilot phase and related data, as well as the concepts of similitude. Special attention should be paid to the detailed engineering of the possible technical solutions. Depending on their nature, the models can either provide a description of how the system behaves in certain conditions or be used to calculate the detailed geometric measures of the equipment. For example, we show that all the dimensions of a distillation column can be calculated when we definitively establish the separation requirements. Special consideration should be given to the process of scaling-up, because here we must appreciate whether the same phenomena occur identically occur on both scales (see Chapter 6 for similitude laws). Similarly, when equipment is being scaled up, attention should be paid to its parameters, because they can be a function of the size. When dealing with empirical models where the origin of the effects is unknown, the uncertainty of the model validity must be considered.

It is useful to have detailed documentation concerning all the assumptions and theories used in the model. The yield and energy consumption of a process are easily optimised using fine-tuned models to design a new unit or process. Depending on the process integration, pinch analysis and other similar analysis procedures can be used to find a solution of heat integration. Various data on streams and energy consumption, which are easily developed from simulation results, can be used to sustain the adopted technical solutions.

1.3.5
Modelling and Operating Stage

At this stage of the process life-cycle, the models must include all relevant physical, chemical and mechanical aspects that characterize the process. The model predictions are compared to actual plant measurements and are further tuned to improve the accuracy of the predictions. This consideration is valuable, especially for the finally adjusted models that create the conditions of use to meet the demand of this operating stage so as to guarantee optimal production. Models can also be used in many ways in order to reduce the operating costs. In the mode of parameter estimation, the model is provided with the process measurement data reflecting the current state of the process, which makes it possible, for example, to monitor the fouling of a plant heat exchanger. Once the heat transfer coefficient falls under a preset limit, it is time for maintenance work. In this way a virtual process can be kept up to date.

In simulation mode, the performance of the process can be followed. Discrepancies between the model and the process may reveal instrumentation malfunction, problems of maintenance etc. Verified flow-sheet models can be used to further analyse the process operation. In the optimising mode, the models are especially used when different grades of the product are manufactured with the process. At this point we criticize the old practices that rely on the tacit knowledge of an experimented operator and consider the models as an artificial creation, which cannot attain the operator's performance.

The importance of storing process data has been emphasized here. After all, the data are an important link in the creation cycle of the process knowledge. Future applications concerning the gathering of new data will provide a powerful tool in the use of the stored data or process memory. It is important to keep in mind that, at this stage, the process could be further improved as new ideas, capacity increasing spin-off projects, R&D projects, etc. are developed. These developments frequently require a partial implementation of the methodology described above. Therefore, the models of the existing process could act as a tool in further developments.

In practice, models are often tailor-made and their use requires expertise. Building interfaces, which take into account the special demands arising from man–computer interaction, can greatly expand the use of the models.

Table 1.1 summarizes the discussions on the modes under which the models are used, which are explained in Sections 1.1–1.3.

Table 1.1 The modes of model use for all the stages in the life-cycle process.

Mode	Input models data	Computed (exit) models data
Simulation	values of input process variables values of process parameters values of non-process parameters	values for exit process variables
Design	values of input process variables values of exit process variables values of non-process parameters	values of process parameter (those that show the equipment size)
Parameter estimation	values of input process variables values of exit process variables values of process parameters	values of non-process parameters
Optimization	all fixed input process variables – all fixed exit process variable – all process non-parameters – some fixed process parameters – optimization expressions	optimal non-fixed inputs optimal non-fixed exits – optimal non fixed parameters – values of optimized functions

Concerning the question *Why modelling*?, which is also the title of this chapter, we can assert that the use of models is important because these have the capacity to assist the solution of many important and fundamental problems in chemical engineering.

We can especially mention that modelling can be successfully used to:

- reduce manufacturing costs
- reduce time and costs in all stages of the process life-cycle
- increase process efficiency
- allow a better and deeper understanding of the process and its operation
- be used as support for the solutions adopted during the process development and exploitation
- ensure an easy technological transfer of the process
- increase the quality of process management
- reveal abilities to handle complex problems
- contribute to reducing pollution
- improve the safety of the plants
- market new products faster
- reduce waste emission while the process is being developed
- improve the quality of the products
- ensure a high quality of training of the operators.

1.4
Actual Objectives for Chemical Engineering Research

In the past, the scope of chemical engineering research ranged from process engineering to product engineering. It was firstly defined as the capacity to produce one chemical product with complex designed properties. It was occasioned by the necessity to produce one profound transformation of the existing chemical production systems. The objective then was to produce the state displacement in the vicinity of its thermodynamic efficiency [1.19, 1.20]. Many theoreticians and practitioners accept that if the researcher wants to obey all the statements described above, changes in many of the classical research procedures are required [1.21, 1.22].

Trying to discover the basic concepts that will be the keys to successful applications in the future, more and more scientists consider that the chemical engineering design and research must meet five major objectives [1.23–1.26]:

1. *The first objective* is represented by the need to increase the productivity and selectivity of both existing and new processes through intelligent operations and multiscale control of processes. This objective is sustained by the important results obtained thanks to the synthesis of a new class of engineered porous supports and catalysts. So the catalytic reactions and separation processes that use these materials can be efficiently controlled.

   Microtechnology makes it possible to produce these materials in series. Other materials with a controlled structure begin to be developed for chiral technologies.

Such approaches imply that chemical engineers should go down to the nanoscale to control events at the molecular level. At this level, manipulating supramolecular building blocks can create new functions in interacting species such as self-organization, regulation, replication and communication. Consequently a new mathematical characterisation must be produced and used to describe these discrete functions.

At the microscale level, detailed local temperature and composition control through the staged feed and supply of reactants or the removal of products would result in a higher selectivity and productivity than would the conventional approach. Indeed, this conventional approach imposes boundary conditions and lets a system operate under spontaneous reaction and transfer. To produce a local energy supply, microwave and ultrasound can be used instead of heat. To operate the relevant models on these energies, local sensors and actuators as well as close computer control will absolutely be needed.

On the other hand, on-line information on the process state and on the quality of the products should not be limited to such usual parameters as pressure, temperature, pH and composition, but should extend to more sophisticated characteristics such as colour, smoothness, odour, etc. To produce and to introduce these parameters into the current production in progress, modelling and experimental research must be combined.

2. *The second objective* is represented by the need to design novel equipment based on scientific principles corresponding to novel modes of production.

   We cannot begin a short discussion about this objective without observing that despite new technological and material developments, most of the equipment used in chemical plants is based on 100-year old principles. On the other hand, past research in chemical engineering has led to a better understanding of the elementary phenomena and now we can conceive novel equipment based on these scientific principles.

   Apparently, it is not difficult to imagine coupling a chemical reaction with separation or heat transfer to obtain a concept of multifunctional reactors which frequently result in higher productivity.

   The scientific design of the novel equipment and of the new modes of production is also sustained by new operating modes used on the laboratory scale, such as reversed flow, cyclic processes, unsteady state operation, extreme operating conditions (very high pressure and temperature) as well as supercritical media processing. These new modes of production have proved their efficiency and capacity to be modelled and controlled.

Current production modes may also be challenged by miniaturization, modularisation, and decentralization. Recently developed microtechnologies using microreactors, microseparators and very small microanalysers show new possible ways to accurately control reaction conditions with respect to mixing, quenching and temperature profiles. These microtechnologies show that the scientific design of novel equipment begins to be a reality. Such innovative systems can be applied if these novel technologies prove to be robust, reliable, safe, cheap, easy to control, and if they provide significant gains over existing processes.

3. *The third objective* is the need to manufacture chemical products with imposed end-use properties. The consideration of this objective is given by the present and prospective market demand.

   There is indeed a growing market demand for sophisticated products combining several functions and properties. As examples, we can mention coatings, cosmetics, detergents, inks, lubricants, surfactants, plastics, food, agrochemicals, and many more products the basic function of which has been excluded while two or more characterizing functions have been identified. In the past, most formulation recipes have resulted from experiments and empirical tests. A good knowledge of the characteristics of such complex media as non-Newtonian liquids, gels, foams, hydrosoluble polymers, dispersions and suspensions can be the key to revolutionizing the design of such products. At the same time, rheology and interfacial phenomena can play a major role in this design.

   The prospective market shows signs indicating a great demand for special solids which can act as vehicles conveying condensed matter: this particular property is one of the most frequently demanded. These products can open the way to solvent-less processes. These so-called intelligent solids, presenting controlled reactivity or programmed release of active components, may be obtained through multiple coating on a base solid. All the operations that are related to the manufacture of these products must be reanalysed and reconsidered with respect to the micro- and nanoscale evolution. Particle-size distribution and morphology control are the central concerns in such operations as precipitation, crystallization, prilling, generation of aerosols, and nanoparticles. Agglomeration, granulation, calcination, and compaction as final shaping operations need better understanding and control.

Several questions are raised by the overall problem of manufacturing chemicals with multifunctional properties: how can the operations be scaled-up from the laboratory model to an actual plant? Will the same product be obtained and its properties preserved? What is the role of equipment design in determining the properties of the products? These questions are strongly sustained by the fact that the existing scaling-up procedures cannot show how such end-use properties such as colour, flowability, sinterability, biocompatibility and many others can be controlled.

4. *The fourth objective* includes the need to use multiscale computational chemical engineering in real-life situations.

   The computer applications of molecular modelling using the principles of statistics and quantum mechanics have been developed successfully. They are a new domain for chemical engineering research. Some basic characteristics of the materials' interaction can be calculated by molecular modelling based on information from data banks.

   Dynamic process modelling is being developed to be used on the macroscopic scale. Full complex plant models may involve up to 5.0×10^4 variables, 2.0×10^5 equations and over 1.0×10^5 optimisation variables.

   It is important to avoid confusion between modelling and numerical simulation. Modelling is an intellectual activity requiring experience, skills, judgment and the knowledge of scientific facts. For example, the main obstacle to developing good models of multiphase and complex systems consists more in understanding the physics and chemistry of all interactions than refining the numerical codes of calculations.

   Actually, a model could be divided into smaller units. For example, a global production unit could be divided into catalyst particles, droplets, bubbles, etc, and this could even be extended up to discrete molecular processes.

5. *The fifth objective* concerns the need to preserve the environment. This objective requires the use of non-polluting technologies, the reduction of harmful emissions from existing chemical sites and the development of more efficient and specialized pollutant treatment plants.

We can see that the above-mentioned objectives clearly show that, when one research problem has been fixed, the solution has to be reached taking into consideration the strong relation between the modelling and the experimental research. First both modelling and simulation must indicate the type of experiment needed for a thorough knowledge of the phenomenon. Then, the modelling must identify the best conditions for the evolution of the process phenomena. Complex models with a high hierarchy and complex part connections followed by more and more simulations can contribute to the success of this modern type of chemical engineering research.

1.5
Considerations About the Process Simulation

From the sections above, the reader can observe that the notion of a chemical process can be quite complex. The chemical reactions that take place over a broad range of temperatures and pressures are extraordinarily diverse. From the modelling viewpoint, this complexity results in a considerable number of process and non-process parameters with an appreciable quantity of internal links, as well as in very complex equations describing the process state (the relationships between input and output process variables).

When we build a model, some phenomena are simplified and consequently some parameters are disregarded or distorted in comparison with their reality. In addition, some of the relationships between the parameters could be neglected. Two ways of controlling the output or input of information are available in model building: (i) the *convergence way* which accepts the input or output information only if it preserves or accentuates the direction of the evolution with respect to the real modelled case; (ii) the *divergence way* in which we refuse the input or output of information because it results in a bad model response. To identify the direction of the model response to an input or output of information, we need to realize partial model simulations adding or eliminating mathematical relations from the original model architecture. In Table 1.1 we can see a final process model which is used for the exploitation of the process in the simulation or optimisation mode for an actual case.

One of the answers to the question *Why modelling?* could therefore be the establishment of a set of simulation process analyses. In addition to the mathematical simulation of processes described above, we have the simulation of a physical process, which, in fact, is a small-scale experimental process investigation. In other words, to simulate a process at laboratory-scale, we use the analysis of a more affordable process which is similar to experimental investigation.

1.5.1
The Simulation of a Physical Process and Analogous Computers

The simulation of a physical process consists in analysing the phenomena of the whole process or of a part of it. This is based on the use of a reduced-scale plant, which allows a selected variability of all input variables. We have to focus this analysis on the physical particularities and on the increase in the dimensions of the plant. We then treat the obtained experimental data in accordance with dimensional analysis and similitude theory (for instance, see Chapter 6). The dimensionless data arrangement, imposed by this theory, creates the necessary conditions to particularize the general similitude relationships to the analysed – physically simulated – case. As expected, these physical simulations are able to reproduce the constant values of dimensionless similitude criteria in order to scale-up an experimental plant into a larger one. Then, it makes it possible to scale-up the plant by simply modifying the characteristic dimensions of each device of the experimental plant.

At the same time, when we impose the dimensions of the plant, we can focus on obtaining one or more of the optimal solutions (maximum degree of species transformation, minimum chemical consumption, maximum degree of species transformation with minimum chemical consumption etc.) For this purpose, it is recommended to use both mathematical and physical simulations.

For physical process simulation, as well as for mathematical model development, we can use the *isomorphism* principle. This is based on the formal analogy of the mathematical and physical descriptions of different phenomena. We can detail this principle by considering the conductive flux transport of various properties, which can be written as follows:

$$\text{for momentum transport} \qquad \tau_{yx} = -\eta \frac{dw_y}{dx} \tag{1.4}$$

$$\text{for heat transport:} \qquad q_x = -\lambda \frac{dt}{dx} \tag{1.5}$$

$$\text{for species A transport:} \qquad N_{Ax} = -D_A \frac{dc_A}{dx} \tag{1.6}$$

$$\text{for electric current transport:} \qquad i_x = -\frac{1}{\rho} \frac{dU}{dx} \tag{1.7}$$

It is not difficult to observe that in all of these expressions we have a multiplication between the property gradient and a constant that characterizes the medium in which the transport occurs. As a consequence, with the introduction of a transformation coefficient we can simulate, for example, the momentum flow, the heat flow or species flow by measuring only the electric current flow. So, when we have the solution of one precise transport property, we can extend it to all the cases that present an analogous physical and mathematical description. Analogous computers [1.27] have been developed on this principle. The analogous computers, able to simulate mechanical, hydraulic and electric micro-laboratory plants, have been experimented with and used successfully to simulate heat [1.28] and mass [1.29] transport.

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