2
On the Classification of Models

The advances in basic knowledge and model-based process engineering methodologies will certainly result in an increasing demand for models. In addition, computer assistance to support the development and implementation of adequate and clear models will be increasingly used, especially in order to minimize the financial support for industrial production by optimizing global production processes. The classification of models depending on their methodology, mathematical development, objectives etc. will be a useful tool for beginners in modelling in order to help them in their search for the particular model able to solve the different and variable products synthesis.

Highly-diversified models are used in chemical engineering, consequently, it is not simple to propose a class grouping for models. The different grouping attempts given here are strongly related to the modeled phenomena. In the case of a device model or plant model, the assembly of the model parts creates an important number of cases that do not present any interest for class grouping purposes. In accordance with the qualitative process theory to produce the class grouping of one phenomenon or event, it is important to select a clear characterization criterion which can assist the grouping procedure. When this criterion is represented by the theoretical base used for the development of models, the following classification is obtained:

- mathematical models based on the laws of transport phenomena
- mathematical models based on the stochastic evolution laws
- mathematical models based on statistical regression theory
- mathematical models resulting from the particularization of similitude and dimensional analysis.

When the grouping criterion is given by the mathematical complexity of the process model (models), we can distinguish:

- mathematical models expressed by systems of equations with complex derivatives
- mathematical models containing one equation with complex derivatives and one (or more) ordinary system(s) of differential equations

Chemical Engineering. Tanase G. Dobre and José G. Sanchez Marcano

ISBN: 978-3-527-30607-7

- mathematical models promoted by a group of ordinary systems of differential equations
- mathematical models with one set of ordinary differential equations complete with algebraic parameters and relationships between variables
- mathematical models given by algebraic equations relating the variables of the process.

For the mathematical models based on transport phenomena as well as for the stochastic mathematical models, we can introduce new grouping criteria. When the basic process variables (species conversion, species concentration, temperature, pressure and some non-process parameters) modify their values, with the time and spatial position inside their evolution space, the models that describe the process are recognized as *models with distributed parameters*. From a mathematical viewpoint, these models are represented by an assembly of relations which contain partial differential equations The models, in which the basic process variables evolve either with time or in one particular spatial direction, are called *models with concentrated parameters*.

When one or more input process variable and some process and non-process parameters are characterized by means of a random distribution (frequently normal distributions), the class of *non-deterministic models* or of *models with random parameters* is introduced. Many models with distributed parameters present the state of models with random parameters at the same time.

The models associated to a process with no randomly distributed input variables or parameters are called *rigid models*. If we consider only the mean values of the parameters and variables of one model with randomly distributed parameters or input variables, then we transform a non-deterministic model into a rigid model.

The stochastic process models can be transformed by the use of specific theorems as well as various stochastic deformed models, more commonly called *diffusion models* (for more details see Chapter 4). In the case of statistical models, we can introduce other grouping criteria. We have a detailed discussion of this problem in Chapter 5.

In our opinion, one important grouping criterion is the chemical engineering domain that promotes the model. In the next section, modeling and simulation have been coupled and a summary of this classification is given.

2.1 Fields of Modelling and Simulation in Chemical Engineering

Some important chemical engineering modelling and simulation fields as well as related activities are briefly presented here. First, we can see that the traditional modelling procedures or *computer-aided process engineering* cover a much narrower range of modelling tools than those mentioned here. A broader spectrum of chemical engineering modelling and simulation fields is developed and illustrated elsewhere in this book.

2.1.1 Steady-state Flowsheet Modelling and Simulation

Process design for continuous processes is carried out mostly using steady-state simulators. In steady-state process simulation, individual process units or entire flowsheets are calculated, such that there are no time deviations of variables and parameters. Most of the steady-state flowsheet simulators use a sequential modular approach in which the flowsheet is broken into small units. Since each unit is solved separately, the flowsheet is worked through sequentially and iteration is continued until the entire flowsheet is converged. Another way to solve the flowsheet is to use the equation oriented approach, where the flowsheet is handled as a large set of equations, which are solved simultaneously.

Flowsheet simulators consist of unit operation models, physical and thermodynamic calculation models and databanks. Consequently, the simulation results are only as good as the underlying physical properties and engineering models. Many steady-state commercial simulators [2.1, 2.2] have some dynamic (batch) models included, which can be used in steady-state simulations with intermediate storage buffer tanks.

2.1.2 Unsteady-state Process Modelling and Simulation

Unsteady-state or dynamic simulation accounts for process transients, from an initial state to a final state. Dynamic models for complex chemical processes typically consist of large systems of ordinary differential equations and algebraic equations. Therefore, dynamic process simulation is computationally intensive. Dynamic simulators typically contain three units: (i) thermodynamic and physical properties packages, (ii) unit operation models, (iii) numerical solvers. Dynamic simulation is used for: batch process design and development, control strategy development, control system check-out, the optimization of plant operations, process reliability/availability/safety studies, process improvement, process start-up and shutdown. There are countless dynamic process simulators available on the market. One of them has the commercial name Hysis [2.3].

2.1.3 Molecular Modelling and Computational Chemistry

Molecular modelling is mainly devoted to the study of molecular structure. Computational chemistry is the application of all kinds of calculations, mainly numerical, to the study of molecular structure. It can be considered as a subset of the more general field of molecular modelling because its computations occur as a result of the application of the models.

In contrast to computational chemistry, molecular modelling in the sense of spatial molecular arrangement may not involve any computations [2.4]. Today molecular modelling is being used in an increasingly broad range of chemical systems and by an increasing number of scientists. This is due to the progress made in computer hardware and software, which now allows fundamental and complex calculations on a desktop computer. Computational chemistry is rapidly becoming an essential tool in all branches of chemistry as well as related fields such as biochemistry, biology, pharmacology, chemical engineering and materials science. In some cases, computational chemistry can be used to calculate such compound properties as: shapes – structure and geometry; binding energies – strengths of bonds; charge distributions – dipole, quadrapole, octapole moments; spectra – UV, IR, NMR; thermodynamic properties – energy, entropy, radial distribution functions, structural and dynamic properties – viscosity, surface tension, potential energy surfaces; reaction pathways and energy barriers; product energy distributions and reaction probabilities.

2.1.4 Computational Fluid Dynamics

Computational fluid dynamics (CFD) is the science of determining a numerical solution to governing equations of fluid flow while the solution through space or time is under progress. This solution allows one to obtain a numerical description of the complete flow field of interest. Computational fluid dynamics obtains solutions for the governing Navier–Stokes equations and, depending upon the particular application under study, it solves additional equations involving multiphase, turbulence, heat transfer and other relevant processes [2.5, 2.6]. The partial differential Navier–Stokes and associated equations are converted into algebraic form (numerically solvable by computing) on a mesh that defines the geometry and flow domain of interest. Appropriate boundary and initial conditions are applied to the mesh, and the distributions of quantities such as velocity, pressure, turbulence, temperature and concentration are determined iteratively at every point in space and time within the domain. CFD analysis typically requires the use of computers with a high capacity to perform the mathematical calculations. CFD has shown capability in predicting the detailed flow behaviour for a wide-range of engineering applications, typically leading to improved equipment or process design. CFD is used for the early conceptual studies of new designs, detailed equipment design, scaling-up, troubleshooting and retrofitting systems. Examples in chemical and process engineering include separators, mixers, reactors, pumps, pipes, fans, seals, valves, fluidised beds, bubble columns, furnaces, filters and heat exchangers [2.7, 2.8].

2.1.5 Optimisation and Some Associated Algorithms and Methods

In an optimisation problem, the researcher tries to minimise or maximise a global characteristic of a decision process such as elapsed time or cost, by exploiting certain available degrees of freedom under a set of constraints. Optimisation problems arise in almost all branches of industrial activity: product and process design, production, logistics, short planning and strategic planning. Other areas in the process industry suitable for optimisation are process integration, process synthesis and multi-component blended-flow problems.

Optimisation modelling is a branch of mathematical modelling, which is concerned with finding the best solution to a problem. First, the problem must be represented as a series of mathematical relationships. The best solution to a mathematical model is then found using appropriate optimisation software (solver). If the model has been built correctly, the solution can be applied back to the actual problem. A mathematical model in optimisation usually consists of four key objects [2.9]: data (costs or demands, fixed operation conditions of a reactor or of a fundamental unit, capacities etc.); variables (continuous, semi-continuous, and non-frequently binary and integer); constraints (equalities, inequalities); objective function. The process of building mathematical models for optimisation usually leads to structured problems such as: linear programming, mixed integer linear programming, nonlinear programming and mixed integer nonlinear programming [2.10]. In addition, a solver, i.e. a software including a set of algorithms capable of solving problems, is needed to build a model as well as to categorize the problem. To this end, a specific software can be created but some commercial ones also exist.

Heuristic methods are able to find feasible points of optimisation problems. However, the optimisation of these points can only be proved when used in combination with exact mathematical optimisation methods. For this reason, these methods could not be considered as optimisation methods in the strict meaning of the term. Such heuristic methods include simulated annealing, evolution strategy, constraint programming, neural networks and genetic algorithms. The hybrid approaches combine elements from mathematical optimisation and heuristic methods. They should have great impact on supply chain and scheduling problems in the future.

2.1.6 Artificial Intelligence and Neural Networks

Artificial intelligence is a field of study concerned with the development and use of computer systems that bear some resemblance to human intelligence, including such operations as natural-language recognition and use, problem solving, selection from alternatives, pattern recognition, generalisation based on experience and analysis of novel situations, whereas human intelligence also involves knowledge, deductive reasoning and learning from experience. Engineering and industrial applications of artificial intelligence include [2.11]: the development of more effective control strategies, better design, the explanation of past decisions, the identification of future risks as well as the manufacturing response to changes in demands and supplies. Neural networks are a rather new and advanced artificial intelligence technology that mimic the brain's learning and decision-making process. A neural network consists of a number of connected nodes which include neurons. When a training process is being conducted, the neural network learns from the input data and gradually adjusts its neurons to reflect the desired outputs.

Fuzzy logic is used to deal with concepts that are vague. Many real-world problems are better handled by fuzzy logic than by systems requiring definite true/false distinctions. In the chemical and process industry, the main application of fuzzy logic is the automatic control of complex systems. Neural networks, fuzzy logic and genetic algorithms are also called soft computing methods when used in artificial intelligence.

2.1.7 Environment, Health, Safety and Quality Models

Special models and programs are developed for such purposes as health and safety management and assessment, risk analysis and assessment, emission control and detection and quality control. Such a program may, for example, help the user to keep records regarding training, chemical inventories, emergency response plans, material safety data, sheet expiry dates and so on.

2.1.8 Detailed Design Models and Programs

Certain models and programs are available for the detailed design of processes and process equipment. For example, the process equipment manufacturers often have detailed design and performance models for their products. Engineering design involves a lot of detailed design models.

2.1.9 Process Control

Process control is a general term used to describe many methods of regulating industrial processes. The process being controlled is monitored for changes by means of sensor devices. These sensor devices provide information about the state of the system. The information provided by the sensor devices is used to calculate some type of feedback to manipulate control valves or other control devices. This provides the process with computerized automatic regulation. The essential operations are measurement, evaluation and adjustment, which form the process control loop. Process control systems operate in real-time since they must quickly respond to the changes occurring in the process they are monitoring.

2.1.10
Estimation of Parameters

Parameter estimation for a given model deals with optimising some parameters or their evaluation from experimental data. It is based on setting the best values for the parameters using experimental data. Parameter estimation is the calculation of the non-process parameters, i.e. the parameters that are not specific to the process. Physical and chemical properties are examples of such non-process parameters. Typical stages of the parameter estimation procedure are: (i) the choice of the experimental points, (ii) the experimental work, i.e. the measurement of the values, (iii) the estimation of the parameters and analysis of the accuracy of the results, (iv) if the results are not accurate enough, additional experiments are carried out and the procedure is restarted from stage (i).

In parameter estimation, the parameters are optimised, and the variables are given fixed values. Optimality in parameter estimation consists in establishing the best match between the experimental data and the values calculated by the model. All the procedures for the identification of parameters comply with the optimality requirements [2.12].

2.1.11
Experimental Design

Experimental design (also called "optimal design of experiments" or "experimental planning") consists in finding the optimal set of experiments and measured parameters. A poorly planned experiment cannot be rescued by a more sophisticated analysis of the data. Experimental design is used to maximize the likelihood of finding the effects that are wanted. Experimental design is used to identify or scan the important factors affecting a process and to develop empirical models of processes. These techniques enable one to obtain a maximum amount of information by running a series of experiments in a minimum number of runs. In experimental design, the variables (measurement points) are optimised with fixed parameters.

2.1.12
Process Integration

Process integration is the common term used for the application of system-oriented methodologies and integrated approaches to industrial process plant design for both new and retrofit applications. Such methodologies can be mathematical, thermodynamic and economic models, methods and techniques. Examples of these methods include artificial intelligence, hierarchical analysis, pinch analysis and mathematical programming. Process integration refers to optimal design; examples of these aspects are capital investment, energy efficiency, emissions levels, operability, flexibility, controllability, safety, sustainable development and yields. Process integration also refers to some aspects of operation and maintenance.

Process integration combines processes or units in order to minimise, for example, total energy consumption (pinch analysis). Pinch analysis has been successfully used worldwide for the integrated design of chemical production processes for over ten years. More recent techniques address efficient use of raw materials, waste minimisation, design of advanced separation processes, automated design techniques, effluent minimisation, power plant design and refinery processing [2.13, 2.14]. Responding to their basic principles, the classification of the process integration methods can be given as follows: artificial intelligence / knowledge-based systems; hierarchical analysis / heuristic rules; thermodynamic methods (pinch analysis and energy analysis); optimisation (mathematical programming, simulated annealing, genetic algorithms).

2.1.13
Process Synthesis

Process synthesis tries to find the flowsheet and equipment for specified feed and product streams. We define process synthesis as the activity allowing one to assume which process units should be used, how those units will be interconnected and what temperatures, pressures and flow rates will be required [2.15, 2.16].

Process flowsheet generation is an important part of process synthesis. The following tasks have been established for process flowsheet generation [2.17]: (i) the generation of alternative processing routes, {ii) the identification of the necessary unit operations, (iii) the sequencing of unit operations into an optimal flowsheet.

2.1.14
Data Reconciliation

The main assumption in data reconciliation is that measurement values correspond to the steady state. However, process plants are rarely at steady state. Data reconciliation is used to “manipulate” the measured plant data to satisfy the steady-state assumption. Data reconciliation is used to detect instrument errors and leaks and to get “smoother” data for design calculations.

2.1.15
Mathematical Computing Software

They are the mathematical computing programs that offer tools for symbolic and/or numeric computation, advanced graphics and visualisation with easy-to-use programming language. These programs can be used, for example, in data analysis and visualisation, numeric and symbolic computation, engineering and scientific graphics, modelling and simulation. Examples are Matlab™ and Mathematica™.

2.1.16 Chemometrics

Chemometrics is the discipline concerned with the application of statistical and mathematical methods to chemical data [2.18]. Multiple linear regression, partial least squares regression and the analysis of the main components are the methods that can be used to design or select optimal measurement procedures and experiments, or to provide maximum relevant chemical information from chemical data analysis. Common areas addressed by chemometrics include multivariate calibration, visualisation of data and pattern recognition. Biometrics is concerned with the application of statistical and mathematical methods to biological or biochemical data.

2.2 Some Observations on the Practical Use of Modelling and Simulation

The observations given here are in fact commentaries and considerations about some aspects from the following topics:
- reliability of models and simulations
- role of the industry as final user of modelling and simulation research
- role of modelling and simulation in innovations
- role of modelling in technology transfer and knowledge management
- role of the universities in modelling and simulation development

2.2.1 Reliability of Models and Simulations

Correctness, reliability and applicability of models are very important. For most engineering purposes, the models must have a broad range of applicability and they must be validated. If the models are not based on these principles, their range of applicability is usually very narrow, and they cannot be extrapolated. In many modelling and simulation applications in the process industry, kinetic data and thermodynamic property methods are the most likely sources of error. Errors often occur when and because the models are used outside the scope of their applicability. With the advent and availability of cheap computer power, process modelling has increased in sophistication, and has, at the same time, come within the reach of people who previously were deterred by complex mathematics and computer programming. Simulators are usually made of a huge number of models, and the user has to choose the right ones for the desired purpose. Making correct calculations is not usually trivial and requires a certain amount of expertise, training, process engineering background and knowledge of sometimes very complex phenomena.

The problem with commercial simulators is that, since the simulations can be carried out fairly easily, choosing the wrong models can also be quite easy. Choosing a bad model can result in totally incorrect results. Moreover, with commercial simulators, there is no access to the source code and the user cannot be sure that the calculations are made correctly. The existing commercial flowsheeting packages are very comprehensive and efficient, but the possibility of misuse and misinterpretation of simulation results is high. In CFD and molecular modelling, the results are often only qualitative. The methods can still be useful, since the results are applied to pre-screen the possible experiments, the synthesis routes and to visualise a particular phenomenon.

2.2.2
The Role of Industry as Final User of Modelling and Simulation

This role is not clear, except in the cases of big companies which have their own research and development divisions. In this case, the R&D company division has specialized teams for modelling and simulation implementation. The properly developed models and simulators are then frequently used, as we have already shown, during the life-cycle of all the particular processes or fabrications that give the company its profile. At the same time, each big company's R&D division can be an important vendor of professional software. The small companies that are highly specialized in modelling and simulation, operate as independent software creators and vendors for one or more company's R&D division. The use of modelling and simulation in small and medium size manufacturing companies is quite limited. Since small manufacturing companies and university researchers do not cooperate much, awareness and knowledge about modern Computer Aided Process Engineering tools are also limited. There are of course exceptions among manufacturing companies. Some small and medium size engineering and consulting companies are active users of modelling and simulation tools, which allows them to better justify the solutions they propose to their clients.

2.2.3
Modelling and Simulation in Innovations

Modelling and simulation are usually regarded as support tools in innovative work. They allow fast and easy testing of innovations. The use of simulators also builds a good basis for understanding complex phenomena and their interactions. In addition, it also builds a good basis for innovative thinking. It is indeed quite important to understand what the simulators really do and what the limitations of the models are. As a consequence, access to source codes is the key to the innovative use of models and simulators.

Many commercial programs are usually stuck in old thinking and well-established models, and then, the in-house-made simulators are quite often better innovative tools. Molecular modelling can be used, for example, in screening potential drug molecules or synthesis methods in order to reduce their number.

The existing molecular modelling technology is already so good that there are real benefits in using it. Molecular modelling can be a very efficient and invaluable innovative tool for the industry. The terms “artificial intelligence” and “expert systems” are based on existing knowledge. The *computers* are *not* creative, which means that these tools cannot be innovative. However, they can be used as tools in innovative development work. While most of the modelling and simulation methods are just tools, in innovative work, process synthesis can be regarded as an innovation generator, i.e. it can find novel solutions by itself.

2.2.4
Role of Modelling in Technology Transfer and Knowledge Management

Models are not only made for specific problem solving. They are also important as databases and knowledge management or technology transfer tools. For example, an in-house-made flowsheet simulator is typically a huge set of models containing the most important unit operation models, reactor models, physical property models, thermodynamics models and solver models from the literature as well as the models developed in the company over the years or even decades. Ideally, a in-house-made simulator is a well-organized and well-documented historical database of models and data. A model is also a technology transfer tool through process development and process life cycle (see for instance Fig. 1.5, in Chapter 1). The problem is that the models developed in earlier stages are no longer used in manufacturing. The people in charge of control write simple models for control purposes and the useful models from earlier stages are simply forgotten. Ideally, the models developed in earlier stages should be used and evaluated in manufactoring, and they should provide information to the research stage conceptual design stage and detailed design stage. One reason for “forgetting” the model during the process life cycle is that the simulators are not integrated. Different tools are used in each process life cycle stage. However, simulators with integrated steady-state simulation, dynamic simulation and control and operator-training tools are already being developed. The problem is that the manufactoring people are not always willing to use the models, even though the advantages are clear and the models are made very easy to use.

2.2.5
Role of the Universities in Modelling and Simulation Development

The importance of modelling and simulation for industrial use is generally promoted, in each factory, by the youngest engineers. The importance of computer-aided tools to the factory level is best understood when the application of modelling and simulation has a history. The importance of modelling and simulation is not understood so well in the sectors that do not using computer-aided tools.

Technical universities have a key role in the education of engineers (so that they can work on modelling and simulation) as well as in research and development. In fact, the universities’ education role is absolutely fundamental for the future development of the industry. Indeed, in the future, the work of a process engineer will be more and more concerned with modelling and computation. Moreover, the work will be all the more demanding so that process engineers will need to have an enormous amount of knowledge not only of physics and chemistry, but also of numerical computation, modelling and programming.

References

2.1 *Chemical Complex Analysis System: User's Manual and Tutorial*, MPRI, Louisiana State University, Baton Rouge, 2001.

2.2 *Aspen Plus User's Guide*, Aspen Technology Inc, Cambridge, 1998.

2.3 *Hysis Process User's Guide*, Hyprotech Ltd, Cambridge, 1998.

2.4 J. Leszczynski (Ed.), *Computational Chemistry: Reviews of Current Trends,* Vol. 1–6, World Scientific Publishers, Singapore, 1996–2001.

2.5 K. Srinivas, J. A. C. Fletcher, *Computational Techniques for Fluid Dynamics*, Springer-Verlag, Berlin, 1992.

2.6 D. J. Anderson, Jr., *Computational Fluid Dynamics*, McGraw-Hill, New York, 1995.

2.7 A. J. Robertson, T.C. Crowe, *Engineering Fluid Mechanics*, Wiley, New York, 1996.

2.8 K. V. Garg, *Applied Computational Fluid Dynamics*, Marcel Dekker, New York, 1998.

2.9 G. S. Beveridge, R. S. Shechter, *Optimization Theory and Practice*, McGraw-Hill, New York, 1970.

2.10 M. Tawarmalani, V. Sahinidis, *Global Optimization in Continuous and Mixed-Integer Nonlinear Programming: Theory, Algorithms, Software, and Applications*, Kluwer, Boston, 2001.

2.11 A.B. Bulsari (Ed.), *Neural Networks for Chemical Engineering*, Elsevier, Amsterdam, 1995.

2.12 G. Bastin, D. Dochain, *On Line Estimation and Adaptive Control of Bioreactors*, Elsevier, Amsterdam, 1999.

2.13 B. Linnhoff, D. W. Townsend, D. Boland, G. F. Hewit, B. E. A. Thomas, A. R. Guy, R. H. Marsland, *A User Guide on Process Integration for the Efficient Use of Energy,* The Institute of Chemical Engineering, Rugby, 1992.

2.14 G. Jodicke, U. Fischer, K. Hungerbuhler, *Comput. Chem. Eng.* **2001**, *25*, 203.

2.15 J. M. Douglas, *Conceptual Design of Chemical Processes*, McGraw-Hill, New York, 1988.

2.16 J. Walsh, J. Perkins, *Operability and Control in Process Synthesis* in *Advances in Chemical Engineering, Process Synthesis*, Academic Press, New York, 1996.

2.17 A.W. Westerberg, O. Wahnschafft, *The Synthesis of Distillation-Based Separation Systems* in *Advances in Chemical Engineering, Process Synthesis,* Academic Press, New York, 1996.

2.18 I. D. Massart, G. M. B. Vandeginste, C. M. L. Buydens, S. De Jong, J. P. Lewi, J. Smeyers-Verbeke, *Handbook of Chemometrics and Qualimetrics* (*Parts A and B*), NIR Publications, Chichester, 1997.