CONTROL ENGINEERING LABORATORY
Infotech Oulu
and
Department of Process Engineering

Aspects of process modelling

Juha Jaako

Report A No 6, September 1998

University of Oulu
Control Engineering Laboratory
Report A No 6, September 1998

Aspects of process modelling

Juha Jaako

Abstract: Process modelling is a basic activity in process engineering. The process industries develop and use models for different purposes. This paper, in essence a survey, represents useful model and modelling knowledge categorisations, general requirements set on process models, common modelling paradigms used in process engineering, the phases of the process of process modelling and common modelling pitfalls.

This paper clearly illustrates the manifold approaches or paradigms used in process modelling. It can be argued that these approaches are incompatible with each other and there is a need for general models, that is, models that incorporate more than one modelling paradigm.

Keywords: process modelling, process design, modelling paradigm

Oulu, 11 September 1998 Juha Jaako

ISBN 951-42-5035-4
ISSN 1238-9390
ISBN 951-42-7501-2 (PDF)

University of Oulu
Control Engineering Laboratory
Linnanmaa
FIN-90570 Oulu, Finland

Contents

Founts used: footnotes Tahoma 8 pt, headings Tahoma 10 & 11 pt, text Tahoma 9 pt

1. Introduction

The subject of this short paper is to be an introduction to process modelling.

Before going any further, there is a need for definitions. According to Minsky (1965), we are to use the following definition for a model:

Question: What is a model?
Answer: A model (M) for a system (S) and an experiment (E) is anything to which E can be applied in order to answer questions about S.

This definition does, in fact, tell us nothing about the ingredients of a model. There are many different kinds of models. In process engineering, the same process can be modelled as an experimental set-up in a laboratory, as an abstract set of symbols on a piece of paper, or an collection of ODEs[1], alternately, the process can range from an entire oil refinery to a single drop falling through a gas.

Process modelling is a basic activity in process engineering. The process industries develop and use models, mainly for plant design and operations[2]. Furthermore, almost all areas of process analysis rely on different kinds of process models.

The subject of process modelling is treated somewhat superficially during process engineer's education; Riggs (1988) notes that "It is interesting to note that much of the process engineering curriculum is devoted to developing a quantitative description of physico-chemical systems, yet there is little attention given to the subject of modelling. There is usually some discussion of dynamic modelling as an introduction in process control courses, and some departments offer elective courses in process modelling; but, in general, the chemical engineering graduate does not have a good foundation in the fundamentals of modelling."

One of the biggest problem in process modelling is that many possible models may satisfactorily explain physical phenomena. An example of this aspect is Anscombe's quartet (Edgar 1997), where four data sets are all fitted by least squares to yield the same, simple algebraic model. To sum up, all models are false, but some of these models are useful, and, consequently, it is much easier to prove that a model is false than to prove the opposite.

Models are used to approximate certain characteristics of a process. A model can *never* be a true or an exact representation of a process because it would have to be the same process, or an exact replica, in order to accomplish that. A specific model depends both on the process as well as the application in question. Models constructed for different applications for the same process will therefore differ.

Nilsson (1995) has used following categorisation for different types of models; of course there are numerous other ways to categorise. For every category, there is also a brief description of the use of such approach in process engineering. We have list 1.1.

[1] ODE: ordinary differential equation
[2] For a particular model categorization, see Appendix 1.

List 1.1 Different types of models

- Intuitive[3] - Intuitive models are seldom used, except by their possessors. This is due to the inherent nature of intuitive models, that is, they are inexpressible. Intuitive models find extensive use in process design decisions, plant operations and process control. From plant operations point of view, these models are troublesome because often plant operators have their own more or less false notions (intuitive models) of plant functioning; this can lead to disastrous consequences[4].
- Verbal - If an intuitive model can be expressed in words, it becomes a verbal model; of course causal, qualitative and quantitative models can be simplified by expressing them as a verbal model. When modelling a process, verbal models are almost always used in some, usually initial, stage of modelling. If properly formulated, verbal (or linguistic) models can be transformed into fuzzy models; a sort of qualitative model. Fuzzy models have found extensive use in process engineering lately.
- Causal[5] - As the name implies, these models are about the causal relations of processes.
- Qualitative - Qualitative models are, in a way, a step up in model sophistication. Qualitative models are used when quantitative models are unavailable or too costly to construct. Examples of qualitative models are expert systems, fuzzy models or Qualitative Reasoning (Weld & de Kleer 1990, Bobrow 1984) models. Qualitative models have found applications in diagnosis, process control and scheduling. Qualitative models have, however, inherent limitations, which are pointed out by Woods (1992) using a simple process example.
- Quantitative - Mathematical models are an example of quantitative models. These models can be used for (nearly) every application in process engineering. The problem here is that these models can be too costly to construct, there is not enough knowledge to construct such a model (physical and chemical phenomena are poorly understood), or the application does not really require such model sophistication.

The following questions arise: what is this activity called process modelling and what then is process engineering. Firstly, let us define process engineering[6]; it includes, among other things: (list 1.2)

List 1.2 Process engineering

- Product and process development and design (models are used for describing the chemical physical phenomena in order to better understand the process),
- Process operations monitoring, analysis and diagnosis (the process measurements can be compared with a process model of either a normally operating process or a process with a known fault),
- Process control (predictions of the dynamic short-term behaviour of the process are desired),
- Process optimisation (e.g. fix operational or constructive degrees of freedom),
- Operations planning and scheduling,

---

[3] intuition: (power of) the immediate undestanding of something without conscious reasoning or study.

[4] For example, the infamous Three Mile Island nuclear accident.

[5] causal: of cause and effect; of, expressing, cause

[6] Quite often words *chemical engineering* are used; this is, however, a more restricted definition. The word *chemical* seems to imply that only chemical processes are dealt with.

- Operator training (according to Drengstig *et al.* (1997), a representation solely based on detailed equations is not necessarily the best way to obtain efficient interaction in communicating with other resource personal with different modelling knowledge and background),
- Process hazards analysis,
- Risk assessment, and
- Software engineering for computer-aided engineering environments.

Process modelling is an activity basically using models mentioned in list 1.1 to solve problems in the areas of list 1.2. Process modelling can also be seen as an activity, which uses tools from different scientific disciplines, as described in fig. 1.1.

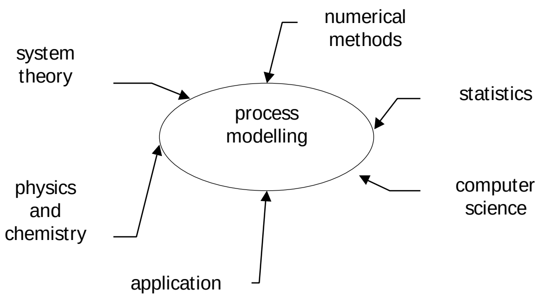

Fig. 1.1. Process modelling tools.

Process modelling *is* understanding of process phenomena and transformation of this understanding into a model.

What is a model used for? Nilsson (1995) presents a generalised model, which, as depicted in fig. 1.2, can be used for different basic problem formulations: simulation, identification (see Ljung 1987), estimation and design. See also (Marquardt 1996).

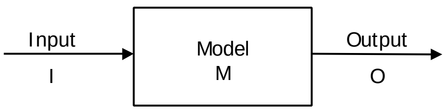

Fig. 1.2. A generalised model.

If model (M) is known, we have two uses for our model:
- Direct: Input (I) is applied on M, output (O) is studied (simulation[7]).
- Inverse: O is applied on M, I is studied.

---

[7] Process models for dynamic simulation are usually in the form of DAE (differential algebraic equations) systems. In order to obtain process models in DAE form some basic assumptions must be made. These general assumptions are usually as follows (Hangos & Cameron 1997):
- Only lumped models are considered.
- Only initial value problems are considered.
- All physical properties in each phase are assumed to be functions of the thermodynamical state variables (temperature, pressure, compositions) only.

With the above assumptions the differential (D) part of the model equations originates from lumped dynamic conservation balances and the algebraic part (A) is of mixed origin; they can be
- Transfer rate expressions,
- Physico-chemical property relations,
- Balance volume relations,
- Equipment and control relations.

If both I and O are known, we have three formulations:

- Identification: We can find the structure and parameters in M.
- Estimation: If the internal structure of M is known, we can find the internal states in M.
- Design: If the structure and internal states of M are known, we can study the parameters in M.

Generally, some demands are set to models; Nilsson (1995) presents a list (list 1.3) of these demands:

List 1.3 Demands set to models[8]

- Accuracy: A requirement placed on quantitative and qualitative models. Do not confuse model accuracy with tool (or programming language) accuracy.
- Validity: We must consider the range of the model[9]. Also consider which operating conditions are applicable; how does the model treat transients; what are the model internal properties.
- Complexity: Models can be simple, usually macroscopic, or detailed, usually microscopic. The detail level of phenomena should also be considered.

Fig. 1.3 shows a comparison of input and output for a process and its model. Note that always n > m and k > t; where n is the number on process inputs, m is the number of model inputs, k is the number on process outputs, and t is the number of model outputs.

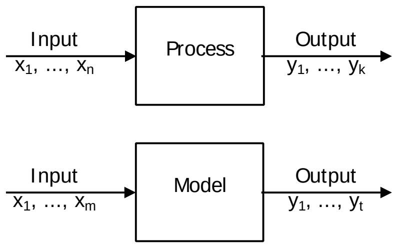

Fig. 1.3. Process vs. process model (Riggs 1988).

In the process industries we can, furthermore, define two levels of models; plant models and models of unit operations such as reactors, pumps, heat exchangers, and tanks.

The state of the art as well as future trends in process modelling can be seen in Marquardt's (1996) paper's references.

[8] Furhermore, we can define yet another demand: quality. The quality of a model is judged by its predictive capability.
[9] A typical process model is non-linear, however, non-linear models are linearised, because they are easier to use. These linear models are valid only in the immediate vicinity of a chosen operating point.

2. Process knowledge available for modelling

When modelling, one should use all accessible knowledge[10] sources. One way to define the task is as follows (Stephanopoulos *et al.* 1996, p. 767)[11]: "It is imperative that we should use models that capture all available knowledge, whether it is expressed in the form of logical propositions, order-of-magnitude, or quantitative relationships." Traditionally, the process engineering discipline has been devoted to quantitative relationships, but during the last ten years it has become possible to model logical propositions (fuzzy models) and order-of-magnitude relationships (qualitative reasoning) in a consistent basis. In the following text, knowledge aspects are treated.

Models can be classified according to the level of the knowledge used (Drengstig *et al.* 1996); list 2.1.

List 2.1 Knowledge levels

- Micro or macro knowledge: Process knowledge is represented on a high[12] level or at a more detailed level. For example, the particle size distribution in a solid material may be described by differential equations at the micro level, or it can be described by a time varying parameter on a macro level.
- Theoretical or empirical knowledge: Model may be based on first principles, or it may be based on an empirical law. First principles knowledge is to be preferred, but it is not always available.
- Explicit or implicit knowledge. Explicit knowledge of a process may, for instance, be given by a mathematical model of the process. If, for instance, only a description of the control system for the process is available, it is possible to say something about how the system behaves, but the knowledge is implicit. Explicit knowledge naturally is to be preferred but it is frequently missing.

Of course, one can find intermediates of these pure extremes.

Leitch (1992) has presented the following figure (Fig. 2.1) to the different attributes inherent to process models and the knowledge connected to them.

[10] A useful book for a reader interested in knowledge engineering is Winston's *Artificial intelligence*.
[11] Compare this with Woods' words in chapter 7.
[12] *Meta-level knowledge* is quite often used instead of *high level knowledge*.

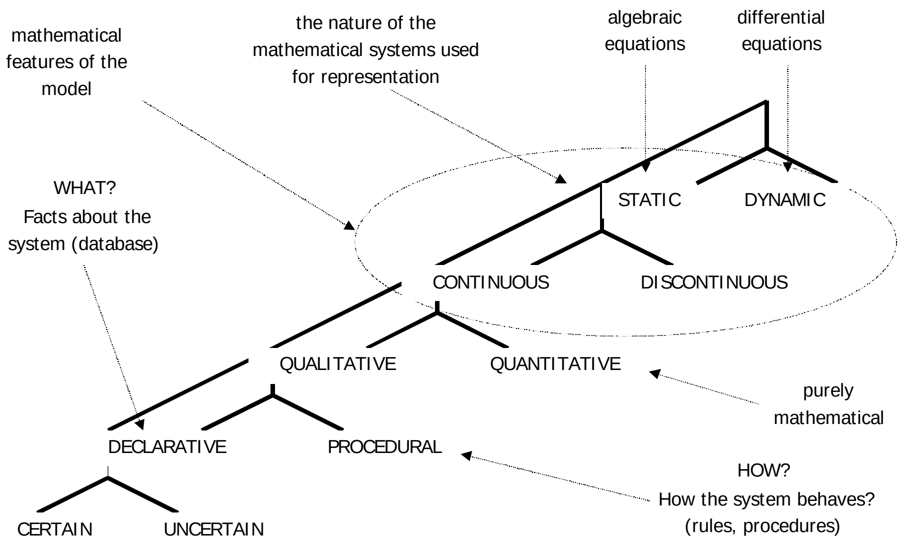

Fig. 2.1. Characteristic dimensions of plant (process) models (Leitch 1992)

Whether a model describes time dependent variations or not, it is classified as dynamic[13] or static, whether the object to be modelled is regarded as a continuum or not, the model is classified as continuous or discontinuous and whether it involves local variations in one or two space variables, it is called one-dimensional or two-dimensional. In addition it can be distinguished between a deterministic and a stochastic description.

If we are not interested in the time dependent behaviour of a process, then a static model will suffice. Predominantly process models are continuous but some processes have discontinuities if not in their time behaviour then in processing order. Qualitative and quantitative dimensions will be treated later in this paper. The uncertainty[14] (which is *always* present) in process models can be of two types. Firstly, we are uncertain whether the values of parameters and initial assumptions are correct or incorrect, and secondly, the knowledge in itself is uncertain, that is, it cannot be proven to be correct or incorrect.

Models can be represented also in three dimensions, list 2.2. One can use the following three axes (Leitch 1992).

List 2.2

- Formal or informal model description: A model may be expressed informally by for instance a textual formulation of the process, or by a rigid formal description. Examples of formal descriptions are mathematical models and formal language (for example, normative) or logic descriptions. Another possible model representation is a graphical diagram. It must be noted, however, that models may be formal and precise in describing one aspect of the process, but at the same time unprecise and informal in other aspects.

---

[13] The concept *dynamic system* means that the current output value depends not only on the current external stimuli but also on their earlier values (Ljung 1987).

[14] The uncertainty associated with parameters used by a model should also be estimated because this will have a direct effect upon overall reliability of the model (Riggs 1988).

- Qualitative or quantitative description: Mathematical models are an example of quantitative models. If there is a need to take into account of the dynamic interactions in a process plant then, according to Woods (1992), we must rely on mathematical models to make predictions about the behaviour of the plant. Examples of qualitative models are expert system descriptions, fuzzy logic descriptions or Qualitative Reasoning (Weld & de Kleer), (Bobrow 1984). Qualitative descriptions are used when quantitative descriptions are unavailable or too costly. Quantitative model types have the following, sometimes opposite, characteristics (Nilsson 1995), see also fig. 2.1.

opposite characteristics	
static	dynamic
lumped	distributed
deterministic	stochastic
continuous	discrete
linear	non-linear
black-box	state-space
time domain	frequency (Laplace) domain

- Procedural or declarative description: A model may be given as a set of procedural steps to follow in order to obtain a solution. A declarative model description does not give any information on how the model should be handled to obtain the solution. The advantage of the latter is, however, that if the procedural description does not fit with the desires of the end-user, the model must be changed, whereas the declarative model may still be applied.

Models can also be classified according to the mathematical point of view. There is a plethora of axes, but below one possibility is listed (see also above).

- Linear or non-linear models: Real world systems are predominantly non-linear. Since linear systems have pleasant mathematical properties, they are preferred in process analysis, control design, etc. Most non-linear systems may be treated as linear near the operating point[15].
- Dynamic or static models: In process analysis, static models are preferred because they are easier and faster to evaluate. Dynamic systems, however, are more difficult to handle, but they gaining more and more acceptance. Algebraic equations (AEs) or partial differential equations (PDEs) describe static systems where the time derivative term has been neglected. Dynamic systems are described by ordinary differential equations (ODEs), differential algebraic equations (DAEs) or PDEs.

[15] As long as the linear models can describe the process behaviour with sufficient accuracy, they are efficient. However, real processes are almost always non-linear, and the engineer needs to content to a linear approximation of the reality, or one needs to turn to non-linear modeling. In non-linear modeling the form of the nonlinearity can be fixed in advance, or model-free estimators can be used to describe complex functions. Typical model free estimators include neural networks and fuzzy systems.

- Lumped or distributed models: In lumped systems the state variables describing the system are lumped in space, in other words, invariant in all spatial dimensions. The system is described by ODEs or DAEs. An example is a CSTR[16]. In distributed systems the state variables vary in one or more directions of spatial co-ordinates. An example is a plug reactor; axial and radial spatial co-ordinates are used. The system is described by PDEs, or even by integro partial differential algebraic equations (IPDAEs) as a general case.
- Continuous or discrete models (Barton & Pantelides 1994): The physicochemical mechanisms that govern the time dependent (dynamic) behaviour of processing systems are predominantly continuous. Modelling of these mechanisms from first principles typically yields large, sparse sets of non-linear equations representing conservation laws, physical constraints, equilibrium, and thermodynamical relationships, and so on. However, few processes can be considered to operate in an entirely continuous manner. Even the majority of 'continuous' processes experience significant discrete changes superimposed on their predominantly continuous behaviour. Such changes typically arise from the application of digital regulatory control, plant equipment failure, or as a consequence of planned operational changes, such as start-up and shutdown, feedstock or product changes, process maintenance, and so on.

Example: For the construction of models in process fault diagnosis, one may tap to the following sources of knowledge:
- Process flowsheets,
- P&I diagrams (a P&I diagram depicts the interconnections of the equipment and instruments of a process together with labels and other data),
- Equipment and instrument specification sheets,
- Event trees and fault trees,
- Operating records,
- Empirical relationships from regressions of data,
- Experience of operating personnel, and
- Principles of chemical engineering science.

The nature of process engineering knowledge is as follows (D'Ambrosio 1990): "Real-world domains are complex to represent. Data are often unavailable or uncertain. Also, there is a difference between theoretical and real-world knowledge. The former is acquired by studying the relevant theory, usually in the form of general laws and axioms. The latter is not acquired through theory: insight is needed into problems that arise in actual situations."

This real world knowledge consists of two different components: deep knowledge and shallow knowledge. Deep knowledge is the set of theoretical laws and axioms that form the basis for abstraction capability. Shallow knowledge cannot be acquired from books; it comes through experience, mentors, blunders, etc.

[16] continuous stirred tank reactor

Example: A good example of working shallow knowledge is the process operator. He performs tasks in the areas of fault diagnosis, planning, process control and process monitoring. Nearly always operator uses only his acquired, shallow knowledge to operate the process; he possesses a mental model[17] of the process. He is, furthermore, capable of maintaining and improving that knowledge. He is, unfortunately, many times unable to explain his actions; that is, his knowledge is implicit, intuitive, and sometimes verbal. Without proper theoretical training, his knowledge level will never reach the level of deep knowledge.

[17] *Mental model* is a model, which does not involve any (mathematical) formalization at all (Ljung 1987). The importance and degree of sophistication of a mental model should not be underestimated.

3. Modelling paradigms

In the following, different types of process modelling paradigms are presented. It should be noted, however, that hybrid approaches (i.e. neural networks and fuzzy models are integrated[18]) are quite common. Furthermore, in many systems, such as chemical and biochemical systems, the modelling task can be divided into two subtasks: modelling of well-understood mechanisms based on mass and energy balances (first-principle modelling), and approximation of partially known relationships such as specific reaction rates.

A good modelling paradigm should be capable to use all the information already available in its different forms. In addition, the resulting model should be simple and easy to comprehend, yet produce accurate predictions.

Mathematical modelling

A mathematical model is a consistent set of algebraic, differential or integral equations describing certain aspects of the behaviour of a system or subsystem (Hofmann 1988). The main advantage of a mathematical model is its ability to predict the course of an event without experimentation, which may be quicker, safer and less costly than experimentation with the real object (if it already exists).

Instead of words *mathematical modelling*, sometimes the words *physical modelling*, misleadingly, are used. The use of words *physical modelling* should be limited to cases when a physical system is used to predict the behaviour of the system of interest (analogue model), for example, an electrical circuit can be used as an analogue model of a mass-spring-dashpot system. Sometimes also words such as *first-principle model*, *phenomenological model or mechanistic model* are used. These models are based on the application of fundamental physical and chemical laws on the system being studied. These fundamental laws include continuity equations (mass, energy and momentum balances), transport phenomena (mass, energy and momentum transport), equilibrium descriptions (phase and chemical equilibrium), kinetic descriptions, and state equations (or descriptions).

Continuity equations are usually in the form of dynamic balances over a system

$$\text{Accumulation} = \text{In} - \text{Out} + \text{Production} - \text{Consumption}$$

A static balance is, of course, of the form

$$0 = \text{In} - \text{Out} + \text{Production} - \text{Consumption}$$

Mass balances are divided into two: component mass balances and total mass balances. A dynamic mass balance of a component in a system is usually expressed in the terms of mole balance instead of mass balance. In dynamic energy balances the accumulation term is the sum of internal, kinetic and potential energies. In chemical engineering, only internal energy is usually considered. Momentum balances are usually discarded, except when the most detailed models are constructed. The transport phenomena are covered in Bird (1976) and Luyben (1973). Kinetic descriptions range from simple relations to quite complicated. Kinetic expressions are very application dependent and particularly when multi-phase systems are modelled. Geometry of the vessels used, possible side-reactions, and inhibitions transform original expressions to something much more complicated in practice.

---

[18] Fuzzy neural networks try to combine the efficient learning methods of neural networks and the simple rule base presentation of knowledge of fuzzy systems.

The formulation of a mathematical model starts with assumptions, the so-called engineering compromises. This stage requires careful consideration; it is correct to list these assumptions for future reference. These assumptions tune the model accuracy, validity and complexity. Next the system descriptions (AEs, ODEs and PDEs) are generated. The next stage is a consistency check, also called model verification. This includes basic checks as degrees-of-freedom analysis; that is, the number of variables equals the number of equations, and units and dimensions check. The next modelling stage transforms the model moderately. This is because the techniques and tools (numerical methods, programming tools) used demand problem formulations on particular form. The last stage is the model verification; the model is tested against data (if available). See also Fug 4.2.

To develop a mathematical model of a process (Drengstig *et al.* 1997, Drengstig *et al.* 1996), some sort of graphical sketch of the process is usually the first step. This graphical sketch is a conceptual picture of the process and the modeller uses it when constructing the mathematical model. Several factors influence the chosen visualisation of the process, e.g.

1. The properties that are believed to be important, e.g. considering a CSTR the most interesting aspects would be the reactions occurring and not the weight of the reaction vessel.
2. Process assumptions like well mixed situation, variable control volume, isolated, closed or open system, the controller structure, possible reactions, or equilibrium.
3. The complexity of the process, i.e. complex phenomena and reactions may be difficult to represent graphically, and hence, have to be represented in some kind of textual or mathematical terms,
4. The purpose of the model, i.e. is it a coarse model of the overall process, or a detailed model of parts of the process, e.g. is it to be used for control or design purposes, or
5. The model format, i.e. the type of model being developed, e.g. mechanistic (analytical) vs. empirical[19] (black box).

The basic steps in mathematical modelling are

- Understanding of mechanistic phenomena and structural connections in the system to be modelled
- *A priori* definition of the degree of sophistication required
- Definition of the dependent and independent variables
- Formulation of the conservation equations, preferentially in dimensionless form
- Specification of the constraints

For the solution of the model, initial and boundary conditions for the variables have to be specified additionally.

[19] Riggs (1988) defines an empirical model as follows: An empirical model assumes the form of the functional relationship between the input and output variables of a process. Then using data from the process, parameters or constants in the functional relationship are determined. Empirical models are best when used in an interpolative manner, but are dangerously unreliable when used for extrapolation.

Models for use in automatic control

Models used for control purposes fall into categories of system modelling, identification, parameter estimation and simulation. See also Nilsson (1995).

- In system modelling models are described in a mathematical framework capturing the system behaviour. This includes linear models (see Ljung 1987 p. 81), continuous models and non-linear models.

  Linear and non-linear systems are generally presented on a state-space form. Linear systems can also be represented as a difference equation in a state-space form. Another possibility is the linear difference equation. There is also a non-linear difference equation.
- In identification models that are fit to measurement data. This includes time series analysis and process identification.

  System identification calls for good experimental data. There is also a choice of model structure; it can be either tailor-made, that is, based on first principles modelling, or ready made, for example an ARX, ARMAX (Auto Regressive, Moving Average, eXtra input, Ljung 1987 p. 73), OE (Output Error model) or BJ (Box-Jenkins) model. Identification methods (beyond the scope of this paper) are numerically demanding, but, luckily, there are ready-made tools, for example, MATLAB Identification Toolbox.
- Parameter estimation uses tailor-made models, ready-made models and physical experiment[20]. Tailor made models are based on first principles and estimation of parameters proceeds with physical interpretation. Ready-made models are general, that is, problem independent (black-box models) and are often stochastic difference equations. Physical experiment based estimation is problem, technology and application dependent. Parameter estimation is usually done with either linear regression methods or iterative methods.

In simulation, models that are generated, are approximated to generate a numerical solution. Methods of model approximation are, for example, space discretization of PDEs to ODEs, linearization of non-linear models to linear models, time discretization of continuous models to discrete models and model reduction. Simulation covers the areas of linear and non-linear equations, sparse matrices and continuous and discrete simulation.

In intelligent control (Årzén & Åström 1995) two paradigms are used, namely, fuzzy control and expert control. Fuzzy control has its roots in manual control. A strong motivation for the approach is the desire to mimic the control actions of an experienced process operator, that is, to model the control actions of the operator. This approach is possible when it is not technically or economically justified to develop a physical or mathematical model. Fuzzy sets, the foundation of fuzzy control, were introduced by Zadeh (1965) as a way of expressing non-probabilistic uncertainties. Also, fuzzy control is no longer only used to directly express a priori process knowledge. For example, a fuzzy controller can be derived from fuzzy model obtained through system identification.

Expert control attempts to represent generic knowledge about feedback control as well as specific knowledge about the particular process, i.e. the knowledge of experienced control and process engineers. This knowledge includes theoretical control

[20] Definitions from Nilsson (1995).

knowledge, heuristics and knowledge acquired during the operation of the process. (Årzén & Åström 1995)

Neural networks

According to Ungar (1996), "neural networks are proving valuable for use in process modelling, optimisation, virtual sensing and control. Neural networks can be called universal multivariable function approximators. More precisely, they can be viewed as multivariate non-linear non-parametric[21] estimation methods: they are typically used to approximate a function $y = f(x)$, where the functional form of f is unknown."

Neural networks[22] have been extensively studied in academia as process models and controllers, and are increasingly used in industry. Neural networks have been used in a variety of different control structures and applications, serving as controllers and process models or parts of process models (e.g. as virtual sensors). They have been used to recognise and forecast disturbances, to detect and diagnose faults, to combine data from partially redundant sensors, to perform statistical quality control, and to adaptively tune conventional controllers such as PIDs.

Neural networks are suitable for non-linear modelling, provided that good-quality measurements are available that describe the process behaviour in the whole operating region.

Then when to use neural networks? Neural networks are attractive models to use when:

- processes are non-linear and
- good first principles (mechanistic) models are not available, either for entire processes or for parts of he process.

However, as Chandrasekaran (1996) has pointed out, for many problems for which neural net techniques are used, other statistical techniques can be used with similar results. This phenomenon can in many instances be attributed to an excess of fascination with mechanisms *per se*.

Fuzzy models

According to Babuška *et al.* (1997), "fuzzy modelling is described as a universal tool for merging first-principle knowledge, measurements and qualitative data from experts." Usually, the following three types of fuzzy models are used: the linguistic (or Mamdani[23]), relational, and Takagi-Sugeno models.

A linguistic fuzzy model is mostly used in capturing qualitative knowledge in the form of if-then rules. This model consists of rules where both the antecedent and the consequent are fuzzy propositions. In fuzzy relational models, a relation represents

---

[21] Neural networks are sometimes called semiparametric methods, to differentiate them from parametric and non-parametric methods. According to Lampinen (1997, p. 29):

- in *parametric* methods the complexity of the model is preselected by the by the number of parameters in the model (i.e., polynomial function fitting or Gaussian density approximation)
- in *non-parametric* methods the number of parameters in the model is determined by the number of training samples (i.e., nearest neighbour methods)
- in *semiparametric* methods the effective complexity of the model is determined by the inherent complexity of the data.

[22] See Lampinen (1997).

[23] Mamdani (1997) & Zadeh (1973)

the mapping between the input and output fuzzy sets. In this model, each rule contains all the possible consequent terms with different weighting factors. This weighting allows us to fine-tune the model, for example, by fitting some data. Takagi-Sugeno model is a mixture of a linguistic and mathematical model. The rule antecedents describe the fuzzy regions in the input space.

According to Babuška *et al.* (1997), fuzzy models can be constructed to emphasise the linguistic and qualitative character or the more analytical character of the description of the process. The former methods are more useful for explanation of the behaviour of the process or the control strategy; the latter are more useful for process analysis and the design of a control strategy. Fuzzy logic is at its best when the target is to automate experimental[24] knowledge expressed in the form of rules.

Babuška *et al.* (1997) have determined the following steps in constructing fuzzy models.

1. The purpose of the model.
2. Determination of a priori knowledge available about the system. Usually there are three different types of process descriptions available: first principle models, models based on measurements, and models based on qualitative knowledge.
3. The structure of the model, that is, the input and output variables.

Example: Fuzzy modelling can be seen, in a way, as modelling of models. For example, the internal process model of an operator is transformed into a fuzzy model. This approach naturally supposes that the original internal model is a correct one, see fig. 3.1.

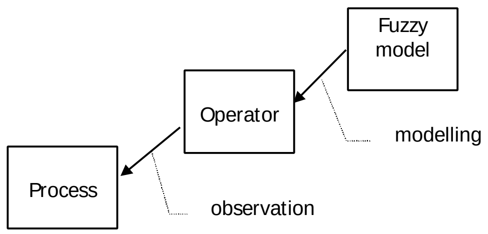

Fig. 3.1. Fuzzy modelling

Fuzzy modelling approach is useful for systems where first principle-based descriptions are difficult to obtain, but partial knowledge about the process and input-output data are available.

Scale models

Scale models are smaller-scale versions of a system, which is usually designed to study one factor. Scale models have the same geometric proportions as the full-scale system but on a smaller scale. A classical example is a wind tunnel in which aircraft designers can analyse the drag of a particular aircraft design using a scale version (model) of the aircraft under specific conditions. Other applications of scale models involve flow modelling and include pilot-scale reactors, small-scale distillation col-

[24] In real industrial processes, measurement data contains noise and is incomplete, containing typically mainly information of the normal operating region.

umns, etc. It should be pointed out, however, that contracting and operating scale models is an expensive activity. See also Riggs (1988).

Modelling of combined discrete/continuous processes

When[25] modelling combined discrete/continuous processes, the modelling task is decomposed into two distinct activities: modelling the fundamental physical behaviour of a processing system, and modelling the external actions imposed on this physical system. Both these activities require discrete components.

Few processes can be considered to operate in an entirely continuous manner. Even the majority of 'continuous' processes experience significant discrete changes superimposed on their predominantly continuous behaviour. Such changes typically arise from the application of digital regulatory control, plant equipment failure, or as a consequence of planned operational changes (start-up, shutdown, feedstock or product changes, process maintenance). Also a common feature of all processing systems is the occurrence of discontinuities in the fundamental physical behaviour. These physicochemical discontinuities typically arise from thermodynamic (phase) and fluid mechanic (laminar → turbulent) transitions, or from geometry of process vessels (non-uniform cross-section). Also external actions, such as opening and closing of manual valves and input ramped between two steady values have mixed discrete (initiation & termination) and continuous (ramping) characteristics.

The are two basically different ways of modelling a combined discrete/continuous system. The first one, proposed by Fahrland (1970), is based on a decomposition into a series of continuous subsystems and discrete subsystems, which are then allowed to interact as equals during the course of simulation. This original decomposition has been reflected in the design of all subsequent combined simulation languages. The second one (Barton & Pantelides 1994) argues that processing systems are more naturally viewed as a single physical subsystem on which external actions are imposed in order to achieve certain objectives. These alternate model decompositions are depicted in fig 3.2.

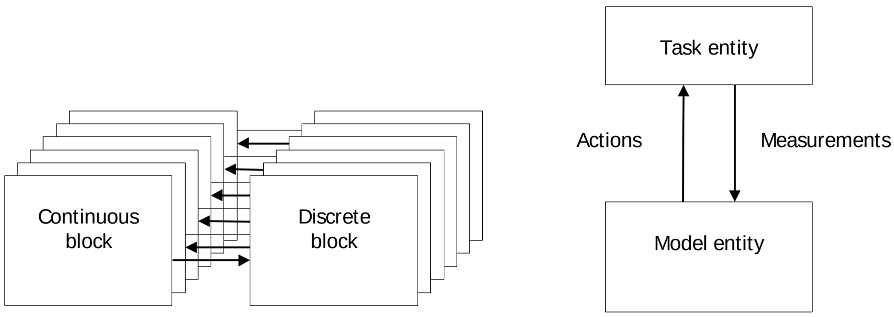

Fig 3.2. Alternate model decompositions.

In fig 3.2 on right *model entity* encapsulates a description of the physicochemical mechanisms governing the behaviour of unit operations and *task entity* encapsulates a description of the control actions of disturbances imposed on this system.

---

[25] This chapter is based on (Barton & Pantelides 1994).

Novel approaches

Most approaches to process modelling concentrate on the purely mechanistic view of a process—in such an extent that other approaches are considered not to exist. There are, however, some frameworks that are also useful in process modelling.

Multilevel Flow Modelling (MFM) (Lind 1990, 1992, Jaako 1996)
Most process representations concentrate on *how* the modelled process is intended to work (process behaviour); less or no emphasis is on *why* this particular behaviour is required; MFM addressed this specific aspect of process modelling.

The formal definition of MFM can be presented as follows: MFM represents functions of an industrial plant by a set of mass, energy, activity, and information flow structures on multiple levels of abstraction. Mass and energy flow structures represent the functions of the plant, and activity and information flow structures represent the functions of the operator or the control system.

The purpose of MFM is to model a system as an artifact, i.e. as a man-made purposeful system. An MFM model is a hierarchical modelling system with two dimensions; these dimensions are called means-ends and whole-part. An MFM model is not a topological model, like a P&I diagram, nor a description of physical structure, it is a functional model; a model which describes the goals, functions and devices of a process. However, a MFM model is a topological model in a sense that it describes the topology of patterns of mass and energy flows and represents qualitative aspects of plant functions in a given operational regime.

The problem in MFM is that model integration is difficult, for example, to integrate MFM with a traditional, mathematical model is inadequate formulated due to the normative nature of MFM[26].

A formal graphical based process modelling methodology (Drengstig *et al.* 1996, 1997)
This is a representation scheme for chemical unit processes. It is based on a topological and phenomenological abstraction of the process. The topological abstraction decomposes the process into control volumes and boundaries. The phenomenological abstraction represents the phenomena in the process using three general process characteristics, i.e. transport, reaction/generation and accumulation of mass and energy[27]. The phenomenological part describes the phenomena taking place inside the topological process components. For these entities, a set of graphical symbols that will be connected together in a network according to the modeller's understanding of the process, giving a representation of the process. These symbols are related to differential and algebraic equations to represent a mathematical model.

This modelling methodology is based on a formal graphical representation scheme. This approach is, in some respects, a similar one as described in Marquardt (1994) and Perkins *et al.* (1994).

The hybrid phenomena theory (HPT, Woods 1992, 1993)
HPT addresses the issue of modelling by integrating both qualitative and quantitative representations. At the quantitative level, HPT employs state-space models to describe the interactions in the process in terms of changing numeric values for vari-

---

[26] That is, models constructed by different persons (of the same object system) will be generally different.
[27] These characteristics are not unlike those of Multilevel Flow Modeling (MFM).

ables. At the qualitative level, a representation describing physical components and interactions in terms of phenomena is used. On top of the qualitative and quantitative layers of the HPT there is a third level, the so-called knowledge level. This level provides a vocabulary for describing the characteristic properties of different kinds of physical interactions.

All these previous representations insert the concept of model hierarchy or model integration or both into the domain of process modelling. For other approaches, see for example Hangos & Cameron (1997), Wasbø & Foss (1996).

4. The process of process modelling

Lohmann & Marquardt (1996) have presented the process of process modelling in a three-dimensional space spanned by the coordinates of specification, representation, and agreement. Here in fig. 4.1 this representation is somewhat simplified.

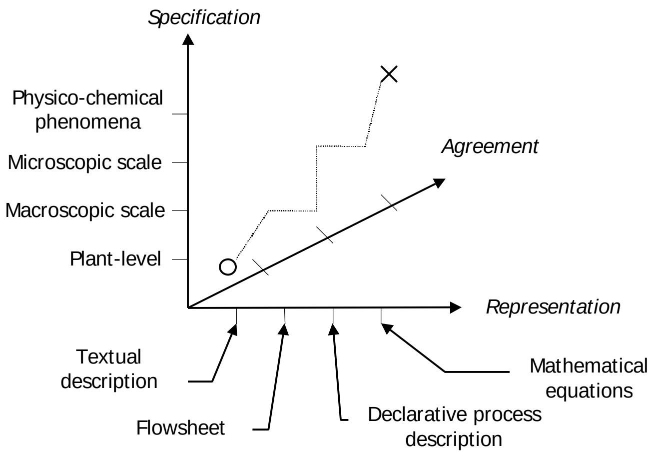

Fig. 4.1 The process of process modelling

The coordinates in fig 4.1 are as follows

- The *specification* dimension relates to the understanding of the model and to the concepts used for process modelling on different levels of granularity. A coarse specification concentrates on the plant level and describes, for example, different sections of a plant. More detail is added on the process unit level. Macroscopic and microscopic scales of specification may be distinguished until all physico-chemical phenomena occurring in the process are finally specified to the required degree of detail.
- The *representation* dimension deals with different formalisms used to express knowledge of the system. Fig 4.1 shows that in the early stages of process modelling typically only informal natural language representations are used. Later on, semi-formal flowsheets and other schematic drawings are added. Finally, the model is represented by mathematical (or other) equations.
- The *agreement* dimension captures the degree of agreement (consensus) reached among different team members (modellers, experts for some unit operations, operating personnel, etc.) involved in a modelling project.

The modelling process can be visualised by a trajectory through this problem space. For example, this trajectory may start in the lower left corner (o, initial state) and end near the upper right corner (x, goal state). The path from the initial to the goal state can be planned (and thus tranformed into a computer program), if all the activities are properly understood. This is, however, not true for process modelling; only parts of the problem space are well understood.

It is, naturally, not necessary always to go all the way to the right in fig. 4.1. For example, textual descriptions can be useful when transformed into a fuzzy model.

General modelling flow diagrams like the one depicted in fig. 4.2 (Marquardt 1996) are quite common. This task sequence is, however, of a too coarse granularity in order to guide the modelling process in adequate detail. To understand the complex modelling process one may decompose every task into elementary modelling steps. Modelling steps can be aggregated to complex modelling procedures to be reused in different contexts. But as the state of knowledge of an object may be sometimes insufficient or limited, modelling can be an iterative process.

Unluckily, there is no single sequence of modelling steps in the sense of a rigid algorithm leading to a certain process model. Rather, depending on the experience and style of the modeler, the modelling steps may be carried out in many valid sequences. The problem for a novice is, however, to know even one valid sequence.

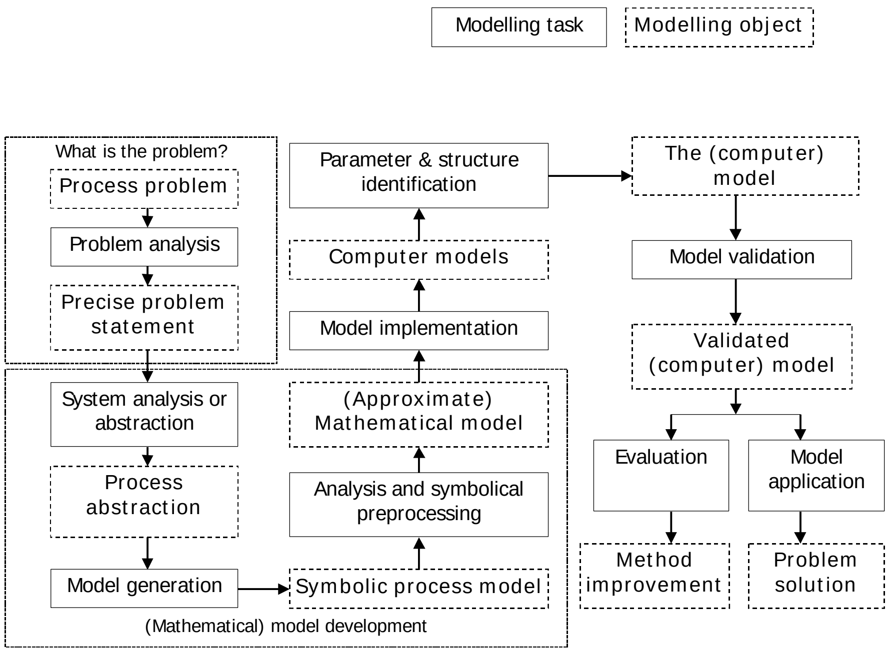

Fig 4.2. Flow diagram of process modelling (Marquardt 1996)

The first task displayed in fig 4.2 is a proper problem analysis to formulate the problem. (Mathematical) model development is accomplished by three distinct but intertwined conceptual tasks with many iteration loops not shown in fig. 4.2. System analysis leads to an informal (verbal or graphical or both) description of the process. Specification of the modelling objects, their behaviour and their aggregation must result in a complete process description, which in turn is used for the generation of symbolic process model. Completeness is, however, impossible to achieve regarding the increasing variety of process units and theories to describe physico-chemical and other phenomena.

After analysis and symbolical pre-processing, the process model is converted into a (sometimes approximate) mathematical model. This in turn is transformed into a numerical algorithm after model implementation. The final modelling tasks are the discrimination of competing model structures and the identification of unknown model parameters as well as the validation of the model. Especially when non-linear models are concerned, all these activities are not sufficiently well understood and supported by adequate methodologies.

The complexity associated with process modelling is usually dealt with the concept of model decomposition, which seems to be the only means to effectively support modelling. This, however, introduces a validation problem because typically only a complete model can be validated for a particular or at best a certain class of applications.

5. Application areas

A useful model provides reliable information about a process from the operating conditions of the process. Process models can be used in following areas (in alphabetical order)

- Equipment maintenance,
- Fault diagnosis[28],
- Planning,
- Process control[29],
- Process design,
- Process monitoring,
- Process optimisation, and
- Scheduling.
- In addition, process models and the development of process models can lead to an overall understanding of the process; i.e., an understanding of the complex interactions within a process.

Some of these areas will be covered in the following. Fault diagnosis is covered in greater detail; it is used as an example. Many of the aspects covered in fault diagnosis are, in fact, common in all application areas.

> Example: Models used for design can be reused in operations. For example, models built to facilitate the design task can be reused for control, optimisation, monitoring, diagnosis, etc. Resources invested in engineering the design process may be repaid in many different ways.

Fault diagnosis

Different process models models for fault diagnosis include quantitative and qualitative models, neural networks and traditional expert systems.

According to Wennersten *et al.* (1996), in order to be of practical use the fault diagnosis system must include a process model which is reasonably correct and complete, transparent to the operator, and flexible for (inevitable) changes in the plant; these are defined in greater detail in table 5.1.

---

[28] In reality, diagnosis is a part of a larger concept, that is, the treatment of plant malfunctions. This can be divided into three basic subtasks: fault localization—monitoring and detection, plant state identification—diagnosis and disturbance compensation—control.

[29] See chapter 3.

Table 5.1 (Wennersten *et al.* 1996)

Word	Definition
Correctness	If the system presents erroneous diagnosis, the operators will soon mistrust its capabilities.
Completeness	Diagnosis must be possible for all situations and parts of the plant. Otherwise it must be clearly stated which application area the system has.
Flexibility for changes	It must be very easy to update the model when something in the process is changed. Changes include plant topology, chemicals used, procedures, etc.
Possibilities to incorporate new knowledge into the system	There must be possibilities to incorporate new experiences from actual deviations that have occurred on the plant site in a flexible way.

Experiences from many systems show that if the model suffers from shortcomings in any of these respects, it will not be used in practise.

In order to construct an operator support system for fault diagnosis, a process model of some kind has to be constructed. This system is usually computerised. The fault diagnosis system should support the operator in finding the root cause to a process deviation. This is somewhat different from alarm analysis, where the logical sequence of several alarms is analyzed. So, the fault diagnosis system should present possible root causes, recommended actions, and possible consequences for different root causes. The problem of finding the consequence of an observed deviation, with identified root cause, is much easier than finding the root cause itself. See Wennersten *et al.* (1996).

Process models for on-line fault diagnosis can be divided into three types: pure heuristic models, deep mathematical quantitative or qualitative models, and statistical models (see Appendix 2). The border between a deep model and a statistical model is not always sharp, as there might be adjustable parameters in the deep model too. The deep model is, however, based upon some concept of basic principles, and contains fewer parameters; additionally, these parameters correspond to identifiable objects.

Fault diagnosis, in its most abstract form, can be defined as a two step model-based task[30]. It can be represented as follows (Stephanopoulos *et al.* 1996):

1. Compare the actual behaviour of a process, as manifested by the values of the operating variables, against the behaviour predicted by a model, and generate the residuals which reflect the impact of faults.
2. Evaluate the residuals and through a model-based inversion process identify the inputs (i.e. faults) that caused the observed behaviour.

[30] The generation of models for fault diagnosis is a fairly complex proposition; especially the validation of the models is quite difficult.

The various approaches that have appeared in the literature (see Stephanopoulos (1996) for an extensive list) are all based on the above simple statement, and they differ in the following aspects:

1. *What sources of faults to consider*; i.e. sensors, actuators, controllers, process equipment, process parameters, or/and operator-induced faults.
2. *What failure modes to include* for each source of faults.
3. *Type of models used to describe process behaviour*; e.g. Boolean, qualitative, order-of-magnitude, quantitative (static or dynamic; deterministic or stochastic).
4. *Representation of process signals*, normally consistent with the type of process models, but not necessarily so.
5. *Computation of residuals*, which are normally (but not always) defined by the type of process models used.
6. *Inversion process*, which could be analytic or take on various forms of a decision process, such as hypothesis testing, logical testing against thresholds, pattern recognition (syntactic, or quantitative), etc.

It is clear that a sound diagnostic approach should be consistent in its choices for all of the above aspects. Actually, the literature is overflowing with diagnostic approaches which have adopted inconsistent positions on the above six aspects, thus leading to and propagating the confusion in this field.

There is a rich variety of models used on fault diagnosis (Stephanopoulos 1996); these include Boolean relationships, directed graphs, order-of-magnitude relationships, qualitative relationships, algebraic relationships for static systems, differential or difference equations, probabilistic and stochastic processes, neural networks, and various rule-based systems. Actually, this richness in the variety of useful knowledge that makes it very hard to develop a generic, all-encompassing methodology for process fault diagnosis.

The diversity of models used on fault diagnosis shows that on the theoretical side there is a need for unification of the diagnostic procedures across different representational models. This unification, although theoretical and conceptual in character, should help researchers and developers to integrate diverse forms of models (diagnostic knowledge) into coherent practical systems.

Process monitoring

Monitoring and diagnosis of process operations has been very fertile ground for the theoretical development and industrial deployment of (intelligent) systems. The framework includes the integration of tools from

- Artificial intelligence (AI) (pattern recognition, rule-based expert systems, fuzzy logic, qualitative simulation (Weld & de Kleer 1990), neural networks, or inductive decision trees),
- Statistical methods (hypothesis testing, principal component analysis, belief networks) and
- System identification techniques (observers, extended Kalman filters, signal analysis).

Process design

The use of process models during the design phase has two incentives (Motard 1996):

- Future operating problems can be caused by oversights during the design process. If at all possible, those problems should be recognised during the design phase. What better framework to confront difficult operating problems, even for operations people who have to deal with problems in plants that have already been built, than a thoroughly engineered and understood "map" of all the entities (static and dynamic) and relations that arise in the description of the plant?
- Sometimes engineers can be so narrowly focused on their speciality areas that they lose sight of the "big picture". Cross-fertilisation between design and operations disciplines is important. Design decision support systems may actually provide that functionality. All of the different perspectives can be considered such as, is the process is easy to start-up and control, does it have low environmental impact during operations, etc.?

In process design models are more useful when used to model the design process. The design process involves (Chandrasekaran *et al.* 1993) exploring design spaces, simulating and verifying candidate designs, and possibly redesigning and repeating the cycle. The modelling object in this case is called design rationale (DR) (*ibid.*). DR includes the body of information that explicitly records the design activity and reasons for making choices (and reasons for *not* making some choices, which is perhaps more important). Research is addressing what kinds of information DR should contain and how to express it. The usefulness of modelling DR is in the fact that the knowledge thus acquired can be used for other modelling purposes; there is no need to start afresh in knowledge gathering (see also chapter 2 and Kaarela (1996)).

There are many approaches useful in this domain, and only some are mentioned here. It should be noted, however, that these approaches are, generally speaking, in their infancy.

- (Chandrasekaran *et al.* 1993): Functional representation (FR) scheme is for causal processes that culminate in the achievement of device functions. FR takes a top-down approach to representing a device in the sense that the overall function is described first and the behaviour of each component is described in the context of this function.
- (Pohjola *et al.* 1994): In this work, methodology of process design is presented as procedural model of how process design is done. Methodology uses object orientation, that is, design project, represented as an object, acts as an adaptive controller of design process.
- Bañares-Alcántara & Ponton (1995) represent a list of functional and representational requirements for a design support system. See also Bañares-Alcántara (1991) for a historical background of this representation.

Planning, optimisation and scheduling

These three application areas, that is, planning, optimisation and scheduling, are intertwined activities. This can be summed up as follows (Reklaitis & Koppel 1996):

- Planning: The allocation of production resources and assignment of production targets for the plant averaged over a suitable time scale, often months or quarters.

- Scheduling/Optimisation: The determination of the timing and sequence in the execution of manufacturing tasks or the selection of operating variable values so as to achieve production targets in a feasible and possibly optimal fashion.

In principle, planning and scheduling are large combinatorial problems, which can be formulated (that is, modelled) as mixed-integer non-linear programming problems. These problems can be solved relatively easily using appropriate software.

Optimisation problems are usually of the form

$$\text{minimise } [G(x,y,z,\ldots)]$$

with constraints

$$h(x,y,z,\ldots) = 0$$

$$g(x,y,z,\ldots) \leq 0$$

where G is usually a cost function (for example, minimise energy losses in a process) and functions h and g are limiting equations (for example, pressure must be below a specific value, there are only two reactors, etc.). A good introductory text for process optimisation is Ray & Szekely (1973).

6. Modelling pitfalls

The modelling project, from the beginning to the end, includes many decisions and compromises. All these acts narrow the scope of the model, and the model becomes a limited representation of the reality, that is, the process. In the following, there are two excerpts from literature, eight years apart. The subject of these is to enumerate common pitfalls in modelling.

According to Riggs (1988), the major pitfalls associated with modelling can listed as follows:

- The controlling factors are not properly identified. In order to identify correctly the controlling factors, you must develop a physical understanding of how the process works; i.e., what factors control the behaviour of the process. This is considered one of the most important steps in the model development process.
- Model validation is lacking. You can never completely validate a model since you can only check your model with a finite number of tests. That is, just because your model passes certain tests does not guarantee that it is correct. Following is a list of approaches that are useful in the search for modelling errors:
    - Verify simplifying assumptions. This involves checking your assumptions using the results of the model, or perhaps even testing the process to examine the accuracy of the assumptions. As an example, consider the assumption of plug flow through a reactor. This assumption can be checked by measuring the outlet concentration profile to an injected slug of tracer for the actual process.
    - Check that the general model behaviour is in accordance with the process behaviour. For example, if the conversion in a reactor increases as the feed rate to the reactor is decreased, the model should show the same behaviour.
    - Develop analytical solutions for simplified cases and compare. For example, if you developed a model for a non-isothermal catalyst particle, it could be checked against the analytical solution for an isothermal case. This validation procedure allows you to check for programming errors and unit conversion errors, as well as the overall physics of your model equations.
    - Compare with other models using common problem. For example, if you had developed a two-dimensional model for a fixed bed reactor, you could compare it with results for a one-dimensional model of a fixed bed reactor by making the appropriate modifications to the input data for your model.
    - Perform a sensitivity analysis to evaluate the effects of parameter uncertainty, that is, you should vary each parameter over its range of uncertainty and observe the resulting effect upon the model predictions.
    - Compare the model directly with process data. This is always the best test of any model. Unfortunately, process data may not be available; e.g. the process does not exist or you may be unable to measure the output variables of the process.
- A model that is incompatible with its end use, is developed.

Jarke & Marquardt (1996, p 98) have pointed out the major shortcomings of the modelling technology (paradigm) routinely used in chemical and process industries:

- Models representations should not only include equations but also operations, model assumptions and limitations (see also chapter Process design).
- Most engineers have problems in formulating non-standard process models.
- Reuse and modification of existing models is not supported.
- The different versions of a model built during a modelling project need to be documented.
- The use of explicit modelling knowledge is not adequate. The modelling experience gathered over time (implicit knowledge) is not stored.
- The libraries of process models are unsatisfactory.

7. In search of general models

There are many ways of modelling a particular process as can be seen it this paper. These ways are, however, mainly incompatible with each other. Two different modelling paradigms can be integrated using an *ad hoc* approach but to use many paradigms in one modelling project in a consistent basis is, it seems, impossible.

The previous phenomenon can be explained as follows. Usually a modeller is restrained by his education and experience to a limited view of a process. Modeller is considering (Jaako 1996 p 39):

- the physical structure of the process (connections between process devices the physical appearance of the process device),
- the functioning of the process (process stages, states and state transformations),
- process flows (mass, energy or information flow),
- process environment (buildings, rooms, etc.)

Or a modeller has in his mind (see Larsson 1992), for example,

- the geographical view of a process,
- the topological view,
- the behavioural view or
- the abstract, hierarchical view.

This all leads to a conclusion that all modelling paradigms start from initial assumptions (views) and a strict adherence to these views makes model integration difficult—see fig. 7.1.

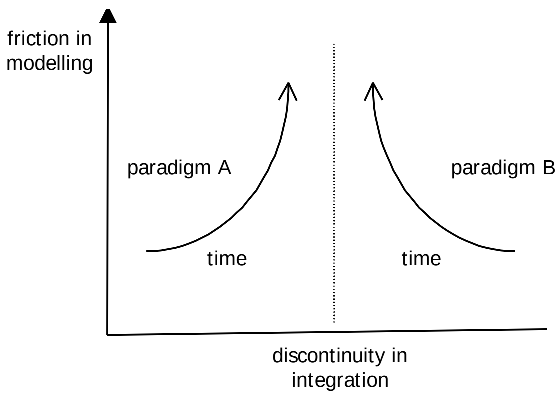

Fig. 7.1 Model integration (*friction* in modelling) (modified from Savolainen 1993)

In essence, the purport of fig. 7.1 is that whatever the modelling paradigm chosen, modelling of a chosen process within that paradigm is relatively effortless; but if the above mentioned views are to be integrated, then the modelling task becomes somewhat involved. Woods (1992) has characterised this phenomenon as follows: "All representations allow us to express some aspects of the system explicitly. Anything, which can be expressed explicitly, is obviously within the expressive power of the representation. Moreover, the model will implicitly describe other characteristic properties of the system or its behaviour. This means that the implicit properties or behaviour can be derived and given an explicit description. But, for a given representation, some properties and behavioural aspects can neither be explicitly described nor derived from any model by any conceivable reasoning methodology. We shall characterise such information as being *beyond the scope of the representation*."

What we need is a representation for a general process model from which we can instantiate current paradigms such as neural networks or first principle models. Jarke & Marquardt (1996) inform us that "advances in process engineering demand models of adequate complexity tailored to the requirements of a variety of application areas. A multi-faceted family of models of *varying degree of detail* is required to adequately support problem solving in its entirety." The problem, naturally, concentrates on how this *varying detail* (*ibid.*) is to be represented.

8. Literature

1. Babuška R, Setnes M, Kaymak U & Verbruggen H B, *Fuzzy modeling: an universal and transparent tool*. Proceedings of TOOLMET'97, Oulu, Finland 1997. pp. 1-27. ISBN 951-42-4648-9.
2. Bañares-Alcántara R, *A Technique to Represent the Design Process of Chemical Plants*. Technical Report 1991-10. University of Edinburgh, Department of Chemical Engineering, 6 pages. (Published in Computer-oriented process engineering, L. Puigjaner & A. Espuña (eds). Elsevier Science Publishers. Amsterdam, The Netherlands. p. 81-86 (1991).)
3. Bañares-Alcántara R & Ponton J W, *Design support systems for conceptual process design*. First International Symposium on Intelligent Systems in Process Engineering, Snowmass, Colorado, July 9-14, 1995. AIChE Symposium Series No 312, Vol 92, p 195-205, 1996.
4. Barton P I & Pantelides C C, *Modeling of combined discrete/continuous processes*. AIChE Journal, Vol 40, No 6, 1994.
5. Bird R B, Stewart W E & Lightfoot E N, *Transport phenomena*. New York 1976.
6. Bishop R H, *Modern control systems analysis and design using Matlab and Simulink*. Addison-Wesley, Menlo Park, Ca., 1996.
7. Bobrow D G (ed), *Qualitative reasoning about physical systems*. North Holland. 1984.
8. Chandrasekaran B, *AI in design: Reviews and prospects*. AIChE Symposium Series No 312, Vol 92, 1996.
9. Chandrasekaran B, Goel A K & Iwasaki Y, *Functional representation as design rationale*. Computer, Vol 26, No 1, pp. 48-56. 1993.
10. D'Ambrosio A, *Modeling real-world processes: Deep and shallow knowledge integrated with approximate reasoning in a diagnostic expert system*. In Artifial Intelligence in Process Engineering, ed. Mavrovouniotis M L, Academic Press 1990. ISBN 0-12-480575-2.
11. Douglas J M, *Conceptual design of chemical processes*. New York, NY, USA, 1988. ISBN 0-07-017762-7.
12. Drengstig T, Wasbø S O & Foss B A, *A formal graphical based process modeling methodology*, Report 96-41-W, NTH Trondheim, Norway, June 1996.
13. Drengstig T, Wasbø S O & Foss B A, *A formal graphical based process modeling methodology*, Comput. Chem. Engng, Vol 21 Suppl., pp S835-S840, 1997.
14. Edgar T F, *Process control - From the classical to the postmodern era*, Chemical engineering education, Vol 31 No 1, Winter 1997.
15. Edgar T F & Himmelblau D M, *Optimization of Chemical Processes*. McGraw-Hill, New York. 1988.
16. Fahrland D A, *Combined discrete event continuous systems simulation*, Simulation, 14, 61 (1970).
17. Fikes R E & Nilsson N J, *STRIPS: A New Approach to the Application of Theorem Proving to Problem Solving*. Artificial Intelligence, Vol 2, 1971.
18. Hangos K M & Cameron I T, *The formal representation of process system modeling assumpions and their implications*. Comput. Chem. Engng, Vol 21 Suppl., pp S823-S828, 1997.
19. Hofmann H, *Future trends in chemical engineering modeling*, Comput. Chem. Engng, Vol 12, No 5, pp. 415-420, 1988.
20. Jaako, J P, *The Extension of Multilevel Flow Modeling*, Acta Univ. Oul. C 87, 1996. ISBN 951-42-4277-7.

21. Jarke M & Marquardt W, *Design and evaluation of computer-aided process modeling tools*. AIChE Symposium Series No 312, Vol 92, 1996.
22. Kaarela K, *Enhancing communication of plant design knowledge*. Espoo 1996. Technical Research Centre of Finland, VTT Publications 272. 110 p + app 81 p. ISBN 951-38-4930-9.
23. Kreyszig E, *Advanced engineering mathematics*. Seventh edition. John Wiley & Sons, New York, 1993.
24. Lampinen J, *Advances in Neural Network Modeling*. Proceedings of TOOLMET'97, Oulu, Finland 1997, pp. 28-35. ISBN 951-42-4648-9.
25. Larsson, J E, *Knowledge-Based Methods for Control Systems*. Ph.D. thesis, Lund Institute of Technology, Department of Automatic Control, Sweden. ISSN 0280-5316, ISRN LUTFD2/TFRT-1040-SE.
26. Leitch R, *Knowledge based control: Selecting the right tool for the job*. Proceedings of IFAC/IFMP/IMACS International Symposium on Artificial Intelligence in Real-Time Control. pp. 25-33. 1992.
27. Leitch R, *Artifial intelligence in control: some myths, some fears but plenty of prospects*. Computing & Control Engineering Journal, July 1992.
28. Levenspiel O, *Chemical reaction engineering*. John Wiley & Sons, New York, 1972.
29. Lind M, *Representing goals and functions of a complex system — An introduction to Multilevel Flow Modelling*. Institute of automatic control systems. Report No: 90-D-381. Technical University of Denmark, July 1990.
30. Lind M, *A categorization of models and its application for the analysis planning knowledge*. Report No: 92-C-433. Technical University of Denmark, 1992.
31. Ljung L, *System identification: Theory for the user*. Prentice-Hall, 1987.
32. Lohmann B & Marquardt W, *On the systematization of the process of model development*. Computers Chem. Engng, Vol. 20, Suppl., pp. S213-S218, 1996.
33. Luyben W L, *Process modeling, simulation and control for chemical engineers*. McGraw-Hill Kogakusha, Tokyo, 1973.
34. Mamdani E H, *Application of fuzzy logic to approximate reasoning using linguistic systems*. Fuzzy Sets and Systems 26, 1182-1191. (1977)
35. Marquardt W, *Trends in computer-aided process modeling*. In: Proc. of PSE'94. Kyongju, Korea, pp. 1-24, 1994.
36. Marquardt W, *Trends in computer-aided process modeling*. Comput. Chem. Engng, Vol 20, No 6/7, pp. 591-609, 1996.
37. Minsky M, *Models, minds, machines*. Proceedings of the IFIP Congress, pp. 45-49, 1965.
38. Motard R & Shum S, *Session summary: Knowledge and CAD environments in engineering design*. AIChE Symposium Series No 312, Vol 92, 1996.
39. Nilsson B, *Process modeling*. PhD Course, Lunds Tekniska Högskola, Lund, Sweden, 1995.
40. Perkins J D, Sargent R W H & Vázgues-Román R, *Computer generation of process models*. In: Proc. of PSE'94. Kyongju, Korea, pp. 123-125. 1994.
41. Pohjola V J, Alha M K, Ainassaari J, *Methodology of process design*. Computers chem. Engng, Vol 18, Suppl., pp. S307-311, 1994.
42. Press W H, Flannery B P, Teukolsky S A & Vetterling W T, *Numerical recipes: The art of scientific computing*. Cambridge, England, Cambridge University Press, 1986.
43. Ray W H & Szekely J, *Process optimization with applications in metallurgy and chemical engineering*. A Wiley-Interscience Publication, 1973.
44. Reklaitis G V, *Introduction to Material and Energy Balances*. Wiley, New York, 1983.

45. Reklaitis G V R & Koppel L B, *Role and prospects for intelligent systems in integrated process operations*. First International Symposium on Intelligent Systems in Process Engineering, Snowmass, Colorado, July 9-14, 1995. AIChE Symposium Series No 312, Vol 92, 1996.
46. Riggs J B, *A systematic approach to modeling*. Chemical Engineering Education, Winter 1988.
47. Savolainen T, *Karkeamallinnusmenetelmä laitostoimituksiin*. Automaatiopäivät 1993, Helsinki. Luentojen lyhennelmät, pp. 160-163. (in Finnish)
48. Stephanopoulos G, *Chemical process control - An introduction to theory and practice*. Prentice/Hall, 1984.
49. Stephanopoulos G & Han C, *Intelligent systems in process engineering: A review*. Computers chem. Engng Vol. 20, No 6/7, pp. 743-191, 1996.
50. Ungar L H, Hartman E J, Keeler J D & Martin G D, *Process modeling and control using neural networks*. AIChE Symposium Series No 312, Vol 92, 1996.
51. Wasbø S O & Foss B A, *Modeling unit processes using formal language description and object-orientation*. Submitted to Mathematical Modeling of Systems, 1996.
52. Weld D S & de Kleer J, *Qualitative reasoning about physical systems*. Morgan Kaufmann, Palo Alto, CA, 1990.
53. Wennersten R, Narfeldt R, Gränfors A & Sjökvist S, *Process modeling in fault diagnosis*. Comput. Chem. Engng, Vol 20, Suppl., pp. S665-S670, 1996.
54. Westerberg A W, Subrahmanian E, Reich Y, Konda S & n-dim group, *Designing the process design process*. Comput. Chem. Engng, Vol 21, Suppl., pp. S1-S9, 1997.
55. Winston P H, *Artificial intelligence*. Addison-Wesley 1993. ISBN 0-201-60086-2.
56. Woods E A, *On representations for continuous dynamic systems*. 1992 IFAC/IFIP/IMACS International Symposium on Artificial Intelligence in Real-Time Control, Delft University of Technology, Delft, The Netherlands, June 16-18, 1992.
57. Woods E A, *The Hybrid Phenomena Theory*, PhD thesis. The Norvegian Institute of Technology. ISBN 82-7119-520-4, 1993.
58. Zadeh L, *Fuzzy sets*. Information and control. 8 (1965), pp. 338-353.
59. Zadeh L A, *Outline of a new approach to the analysis of complex systems and decision processes*. IEEE Trans. Systems, Man, and Cybernetics 1, 28-44 (1973).
60. Årzén K-E & Åström K J, *Expert control and fuzzy control*. First International Symposium on Intelligent Systems in Process Engineering, Snowmass, Colorado, July 9-14, 1995. AIChE Symposium Series No 312, Vol 92, 1996.

Appendix 1

Model categories and their uses in different phases of the plant life cycle (Lind 1992).

	CONTEXT OF USE		
MODEL CATEGORY	PLANT DESIGN	PLANT OPERATION (For implementation of automated and computer supported tasks)	HUMAN-MACHINE INTERFACE (For information presentation, training and plant documentation)
GOAL ORIENTED (appraisive[31])			
What should be achieved	For *specifications* of plant and control system functions.	For *strategic evaluation* of the state of plant and control systems in diagnosis and for hierarchical planning. For setpoint control.	For *functional explanations* and communication of plant and control system *design intentions*.
What should be avoided	For *specification* of functions of engineering plant safety functions and protection systems.	*Strategic evaluation* of safety related plant functions and for emergency management.	For *functional explanations* and communication of design intentions of safety and protection systems.
BEHAVIOUR ORIENTED (designative[32])			
What can be achieved	For *modeling dynamics* of the plant, controllers and safety systems. To be used for simulation and design optimization.	For *estimation* based and adaptive control systems. For *prediction* and *isolation* of the causes of disturbances.	For representation of explanations of plant and control system dynamics, in predictive displays and on- or off-line simulation.
What can go wrong	*Models of* plant, control and safety system *failures*. To be used in risk analysis.	For *fault prediction* in fault disturbance and alarm analysis.	For representation of causes and consequences of plant and control system failures, and in fault prediction displays.
ACTION ORIENTED (prescriptive[33])			
How to achieve goals	Can be used in process and control systems design as heuristics to reduce the complexity of the design problem.	For *decomposition* of plant production goals into control actions.	For *supporting* the operator in the execution of operational procedures.
How to avoid	Can be use in design of safety related plant equipment and protection systems to reduce the complexity of the design problem.	For *decomposition* of safety related goals into protective actions.	For *supporting* the operator in the execution of emergency procedures

Examples:

- Conventional dynamic plant model — behaviour oriented.
- MFM-model — goal oriented.
- Operational procedures (STRIPS - Fikes & Nilsson (1971)), product recipes — action oriented.

---

31 appraise: say what sth is worth
32 designate: mark or point out clearly
33 prescriptive: giving orders or directions

Appendix 2

Heuristic model, a deep mathematical model, and a statistical model (Wennersten *et al.* 1996).

- A heuristic model is a shallow model which describes certain specific phenomena in the process. The process is described in an implicit way through a declarative statement how its function will be under certain conditions. An example of a declarative statement can be as follows: "*If the temperature of a feed stream to a reactor is decreased, then the temperature in the reactor will decrease.*" A common way to represent heuristic knowledge is production rules. These systems are usually referred to as expert systems. The greatest advantage of a heuristic model is that possible root causes for different deviations can be represented in a straightforward way. This approach had its hey-day but there are, however, several serious limitations with this type of heuristic representations (models). Two most important ones are:
    - The knowledge represented is usually only valid under certain conditions which are usually not mentioned. Beyond these conditions, the model is invalid.
    - The plant topology is often implicitly represented in the knowledge statement. If the plant topology is changed, it can be very difficult to update the knowledge in a large knowledge base.

  The systems, which have been built upon traditional expert system technology, have failed because of problems in establishing a complete knowledge base and in adjusting the knowledge base when changes in the process have occurred.

- A deep mathematical model is based on some type of fundamental physical model of the process. This could be e.g. an energy balance or a mass balance for a reaction system. If the model is complete and correct, all specific phenomena could be derived from the model. These models thus constructed can be static of dynamic. Usually these models are quantitative, but a qualitative model can be derived from a quantitative model. A quantitative model will describe qualitative relations between variables, e.g. "*when temperature increases, pressure increases*". For diagnostic purposes this is often sufficient; that is, one must adapt the complexity of the model to the application. In the deep model causality, however, poses some problems. Updating a deep model under constant change concerning plant topology and chemicals used is difficult in a production environment.

- A statistical model is defined as a model without any fundamental physical model of the process. It is a mathematical framework where numerical parameters are fitted to experimental data. An example of this type of model is a neural network; so, a neural network is a statistical model. With this kind of model it is possible to model relations in a process if there is a lot of process data available. The limitations of this model are obvious. It models the process under normal operating conditions. It will not be applicable to find causes to deviations when new situations occur in the process. If the process is changed, the old model is no longer valid, but has to be updated with new process data.

ISBN 951-42-5035-4
ISSN 1238-9390
University of Oulu
Control Engineering Laboratory

Series A
1. Yliniemi L, Alaimo L, Koskinen J, Development and tuning of a fuzzy controller for a rotary dryer. December 1995.
2. Leiviskä K, Simulation in pulp and paper industry. February 1996.
3. Yliniemi L, Lindfors J, Leiviskä K, Transfer of hypermedia material through computer networks. May 1996.
4. Yliniemi L, Juuso E, (editors), Proceedings of TOOLMET'96 - Tool environments and development methods for intelligent systems. May 1996. ISBN 951-42-4397-8.
5. Lemmetti A, Leiviskä K, Sutinen R, Kappa number prediction based on cooking liquor measurements. May 1998. ISBN 951-42-4964-X.
6. Jaako J, Aspects of process modelling. September 1998. ISBN 951-42-5035-4.

OULU UNIVERSITY PRESS
Oulu 1998