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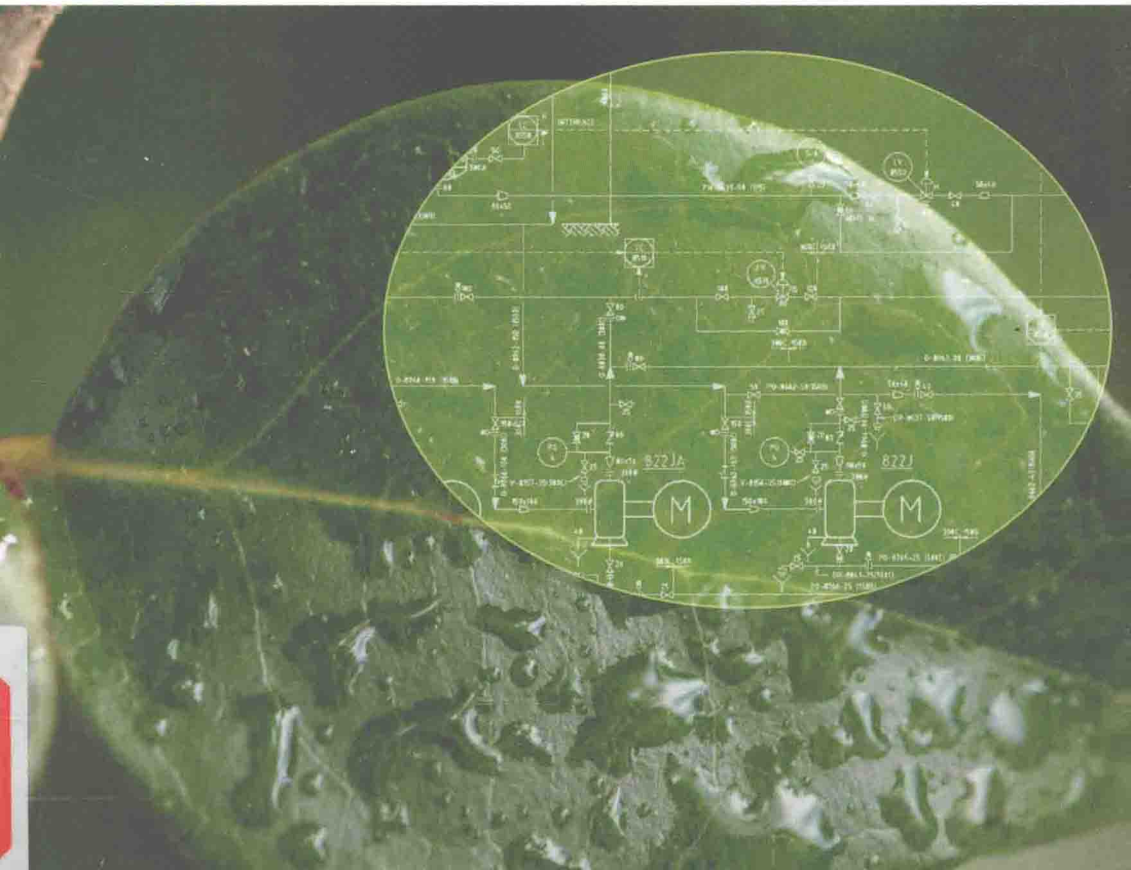
A Case Study Approach



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(continued)

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		7.5	Dynamic polymerisation reactor
		8.3	Short-path evaporation model
		9.1 – 9.2	Tennessee Eastman Challenge Problem
		11.1 – 11.5	Model Identification (Parameter Estimation)
		14.2	ICAS-MoT model library

Preface

This is a case study book on product and process modelling. It has arisen from over 30 years of working in process system applications that required models to be conceptualised, formulated, built and deployed for a range of uses. Modelling is ultimately goal-driven and we are particularly mindful that for modelling "one size does not fit all" applications. We need to be cognizant of the end-goal as we carry out the modelling activity. One thing that has been reinforced over those 30 years is that modelling is a structured activity – we need a modelling methodology to be effective in model building and deployment. Through these case studies you will see that methodology is being exercised across a wide range of modelling applications. Case studies can be a powerful means of understanding how models are formulated, built and used, so we hope this understanding might be enhanced through these examples.

The book is essentially practical in nature, as there are several well-known books that deal with the theory and methodologies that underpin modelling practice. Our intention is not to repeat those ideas but give practical expression to those principles.

To this end, we give a brief coverage of the use and nature of modelling to help set the context of what follows. This includes the practical aspects that are important in modelling and some reflections on the burgeoning availability of modelling tools, many of which can help conceptualise models, provide expert analysis of the properties of the model as well as provide efficient solution of those models. We are now accustomed to seeing large-scale commercial models solved as part of real-time applications in the industry.

The following chapters provide insights into such areas as constitutive models as well as models for steady-state and dynamic applications. We also consider aspects of lumped parameter and distributed parameter modelling via industrial applications drawn from a wide range of industries. There are examples around specific industry sectors which are of current interest. The case studies illustrate the ubiquitous nature of modelling applications and show, in a measured way, just what can be derived from such activities.

In concluding the case studies, we make a number of reflections around the future of product and process modelling – a dangerous activity, given how quickly developments and innovations take place! Not only the benefits from modelling need to be appreciated by practitioners but a real effort needs to be made by practitioners to more effectively communicate the benefits of appropriate modelling and deployment across the product and process life cycle. Much still needs to be done.

Of course this book is the product of many people, not just the principal authors. We are very thankful to the large number of research students who have worked with us over many years in developing methodologies, exercising the principles and applying the resultant modelling to a range of applications. In this matter, we also acknowledge the many industrial supporters of work leading to model development and application. This has been through collaborative research programmes and industrial consulting activities. We thank those who have given permission to present some of this work.

Notably, we would also thank many close colleagues in our academic institutions as well as many in the process systems engineering community worldwide from whom we have benefitted from insights, concepts and practice.

We are hopeful that these case studies will be helpful to many who are in the various stages of the modelling experience – from the novice through experienced practitioner to the expert.

Ian Cameron and Rafiqul Gani

Contents

Chapter 1

Modelling: Nature and Use

This book deals with a broad coverage of modelling concepts and applications for the development of products and processes. It presents these ideas through case studies, showing the importance of modelling to a wide spectrum of discovery activities and decision making processes, that ultimately bring new insights and ideas to reality for social, industrial and economic applications.

There are numerous books and papers available that deal with specific issues in the conceptualisation, development, solution and deployment of models, for applications in many domains of research, business, manufacturing and production. Models are ubiquitous—from those embedded as fuzzy model applications in washing machines through medical applications in anaesthetics, to models that attempt to predict climate variability. Models are routinely used in all areas of human endeavour and appear in various types and forms.

This book presents a number of applications areas, model forms and types, giving insights into some of the important concepts behind modelling, and the drivers for using models in various applications.

1.1. MODELLING FUNDAMENTALS

Modelling in process and product engineering has a long history. It is now clear that much of the design and discovery processes in product and process engineering, are facilitated by various forms of modelling. The decision making processes that are interwoven into the whole of the life cycle, are heavily influenced by modelling, simulation and visualisation.

Modelling, in its minimal form, is the representation of a real or virtual physico-chemical, economic, social or human situation, in an alternate mathematical or physical form, for an envisaged purpose.

This simple definition has three important concepts: an identified system (S) which is the subject of interest, an intended purpose (P) for the model in terms of decision making, and a representational form (M) of the model. The key concepts have associated with them a wide range of issues, relating to details of the system, purpose and form. An extended discussion of such issues can be found elsewhere, as it is not the purpose in this book to dwell on those matters (Aris 1999, Hangos & Cameron 2001).

However, the following sections sketch out some of the key ideas that underpin what is presented in the case studies that appear in subsequent chapters.

1.1.1. Systems Perspectives for Model Development

We need systematic ways of tackling modelling problems. Of particular importance is the application of systems perspectives to modelling activities.

Figure 1 shows a typical systems framework used for conceptualisation of a model. All modelling applications can be cast into such a framework, allowing the modeller to formally describe the system under study. It is equally applicable to the modelling of a complex reactor, as to the interaction model of a human operator with technology, or to the model of active ingredient take-up of sprayed agrochemicals onto a leaf surface. As such, the formalism has a significant descriptive power. The challenge for the modeller is in understanding the individual aspects of the system, which require modelling. Modelling requires significant insight into the system under study.

In Figure 1 a general system (S) with its boundary as the box is given. The states of the system plus inputs, outputs and disturbances, are shown.

The following meaning can be given to the components of the system–

- ***Boundary***: This provides the limits of the model consideration. It is vital to restrict the modelling through a clearly defined boundary. Modelling the behaviour of a single component in a process operation will use a different boundary, to that for a complete production unit.
- Boundaries can also be hierarchical in nature, in that boundaries for lower level detail can be agglomerated into higher levels of view. Likewise, the decomposition of higher level views into finer detail can be achieved as the modelling goal changes.
- ***System:*** The principal entities within the boundary, and their interconnections, including the primary mechanisms operating in that system. The entities can be pieces of processing equipment, phases, people, particles etc.

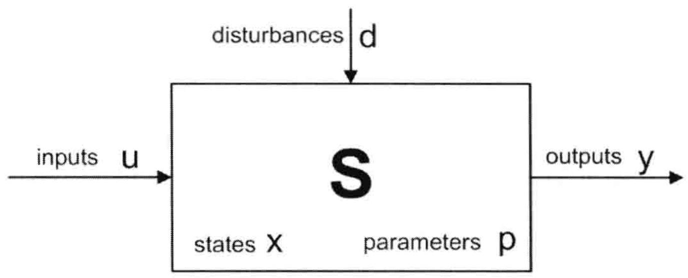

FIGURE 1 A systems perspective for modelling purposes.

- ***States***: These are the variables (**x**) which indicate the 'state' of the system, at a point in time and space. They characterise the important properties of the systems. They are often associated with variables that represent the amount of mass, energy or momentum in a system.
- ***Inputs***: They refer to those variables (**u**) which are associated with the properties of the system that can be chosen to affect the behaviour of the system. They are usually known. They can be flows, temperatures, money, training etc.
- ***Outputs***: They refer to the variables (**y**) that reflect internal properties of the system. They are often linked to the states of the system. They could be production rates, quality measures, target temperatures, efficiencies or any other performance measure of interest.
- ***Disturbances***: They refer to the variables (**d**) that reflect those effects on the system that are normally uncontrolled. They can in some circumstances be measured. These variables could be ambient conditions, raw material quality changes or performance shaping factors affecting people.
- ***Parameters***: They refer to the variables (**p**) that are associated with constants, geometric, physical or chemical properties within the system. In some cases, they can be functions of the states.

The immediate challenge for modelling is to take the real or envisaged situation, and decide what aspects of that reality must be associated with the general systems concepts, so as to answer important questions about the real-world application. This is a 'model conceptualisation' stage.

The action of 'modelling' seeks to replace the real system **S** with a model **M** of sufficient fidelity that will help answer questions about the original system. The required fidelity is often difficult to specify *a priori*, hence leading to iterative activity in the model-building life cycle.

Model conceptualisation involves the decision, about what are the boundaries of the system? How much needs to be captured in the model, in terms of the extent of the system? What are the key mechanisms, and what are the associated system states? What variables will be considered as the inputs, and what will be the outputs that will be an indication of the important performance measures? Can the disturbances be identified, and if so, could they be measured?

These are the initial issues, around capturing the important ideas of the real-world system. However, they are also affected by the modelling goal. Why is this modelling being created, and what will the goal mean for the fidelity and complexity of the model that is needed for a particular application, or range of applications?

1.1.2. Modelling Goals in Applications

Models are developed for a purpose and as suggested in Figure 2, achieving the modelling goal requires a system description, clearly defined application area and the model that represents the real-world phenomena, in sufficient

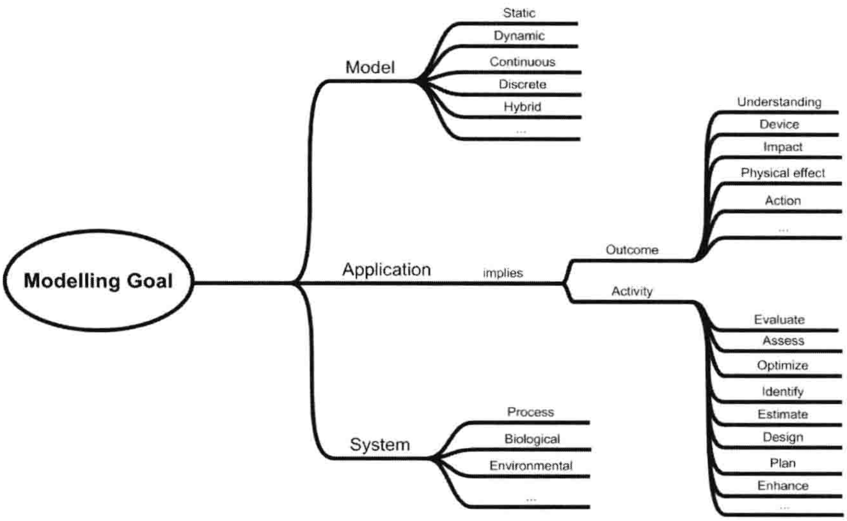

FIGURE 2 Modelling goal components.

fidelity to enable useful questions to be answered. This key focus on the achievable model end-point could be termed 'goal oriented' or 'teleological' modelling.

It was George Box, the famous British statistician and time series modeller who stated that, '. . . all models are wrong, but some are useful . . .'—an excellent truism to bear in mind when building efficient and effective models of real-world systems. There is ultimately an efficiency-thoroughness trade-off that operates when modelling for a purpose (Hollnagel 2009). We need to make decisions about the degree to which we capture system phenomena into the model, and this requires a trade-off between time and ability to provide answers useful in the application of the model. 'Over-kill' in model complexity, is an ever-present challenge for the modeller.

Figure 2 shows that models can have various attributes related to their form and function. This reflects the nature of the underlying phenomena, captured in the model form. The form can reflect the fact that the system is essentially continuous in time and space, or possibly represented by discrete entities such as particles or functions, through discrete actions. The system modelled can be taken from a wide variety of domains in the natural or engineered world, including process, product, economic, biological, human etc.

The model application can be regarded as the combination of a desired *outcome*, and an *activity*, that drives the reason for the modelling in the first instance. Those *outcomes* can relate to *understanding* of the role of complex interactions, in *determining* and *manipulating* behaviour. Hence the activity is clearly an action being carried out, through using the model (evaluate, assess, optimise etc.).

TABLE 1 Model Types and Characteristics

Type of model	Criterion of classification
Mechanistic	based on mechanisms/underlying phenomena
Empirical	based on input-output data, trials or experiments
Stochastic	contains model elements that are probabilistic in nature
Deterministic	based on cause-effect phenomena
Lumped parameter	dependent variables not a function of spatial position
Distributed parameter	dependent variables are functions of spatial position
Linear	superposition principle applies
Nonlinear	superposition principle does not apply
Continuous	dependent variables defined over continuous space-time
Discrete	only defined for discrete values of time and/or space
Hybrid	capturing both continuous and discrete behaviour in the one description

Table 1 gives some further insights into the types and characteristics of models that are often important, in product and process modelling. Section 1.3.2 gives further details of these model types, in the form of a simple classification scheme.

The model types reflect our understanding of the underlying attributes of the system being modelled. All can be observed in the voluminous literature on this topic.

In understanding the modelling goals, we could also classify the major types of generic problems that modelling seeks to answer. The following section sets out a number of such generic problems, commonly addressed by modelling practice.

1.1.3. Typical Problems Addressed by Systems Modelling

The importance of the systems formalism is seen in the various problems that can be tackled, using this generic view. By posing a set of known variables, and leaving others to be estimated, a wide range of important problems are amenable to the use of modelling. These modelling problems include:

1. ***Steady state analysis and simulation***: Given the model of the system **S**, and a fixed operating state $\mathbf{x}_{ss}$ compute the outputs **y**, knowing the inputs **u,** the disturbances **d** and the system parameters **p**. Here the system is regarded as being in 'steady state', or at a particular operating point. Time varying or dynamic behaviour is not being considered here. These types of problems could be identified with standard process flowsheeting applications, or for the use of steady state models in control applications.
2. ***Dynamic analysis and simulation***: Given a model structure for **S**, predict the outputs **y,** knowing the time varying behaviour of the inputs **u**, disturbances **d** and the parameters **p**. This is similar to the previous problem,

except that time varying behaviour is assumed. This type of problem is often focused on assessing the effects of input or disturbance changes, on the outputs of the system. In many cases the combination of steady-state and dynamic models provides profound insights, and even unexpected behaviours, in complex systems.

3. ***The design problem***: In its simplest form: estimate the set of parameters **p**, for a given fixed structure of **S**, desired outputs **y** and specified inputs **u**. Here the situation can be either dynamic or steady state. This problem seeks to find, for example, the size of equipment to give a desired behaviour. There are more complex design problems that require **S** to be found within synthesis problems.
4. ***The optimisation problem***: Estimate the optimum values of the states **x**, for a given objective function F_{obj} involving the states, parameters and inputs. This is a very common application where the 'best' operating point to maximize or minimize some objective, is sought. Unit optimisers in petroleum refineries are a well-known example of such modelling practices.
5. ***Regulatory control or state driving applications***: Estimate the input **u** for a given **S**, **y**, **d** and **p**. This is a standard control issue to obtain the values of the inputs, needed to maintain the system at some specified operating point, or to drive the system from one operating point to another, such as done in batch polymerisation reactors.
6. ***System identification***: Find a structure for the system **S,** with its parameters **p,** using inputs **u** and outputs **y**. This is often done to generate a model to be used for control applications, where the resultant model is embedded into a control algorithm, such as model predictive control (MPC).
7. ***State estimation problem***: Find the internal states **x** of the system **S,** knowing inputs **u** and outputs **y**. This problem is often addressed when there is no direct way to measure the internal state of a system. Through the use of a model and known input and output data, estimates can be obtained using such approaches as Kalman filters.

A number of such applications will be seen, in the case studies presented in subsequent chapters.

1.2. MODEL USE AND DECISION MAKING

Models are widely used in capturing, understanding, investigating and exploiting the aspects of a real-world situation. In the area of product design and development, as well as the invention of processes to make those products, the use of models as decision informing and making tools abound.

1.2.1. Life Cycle Perspectives on Modelling

The extensive nature of model use can be viewed in many ways. A helpful representation that emphasises the breadth and depth of modelling, is seen in

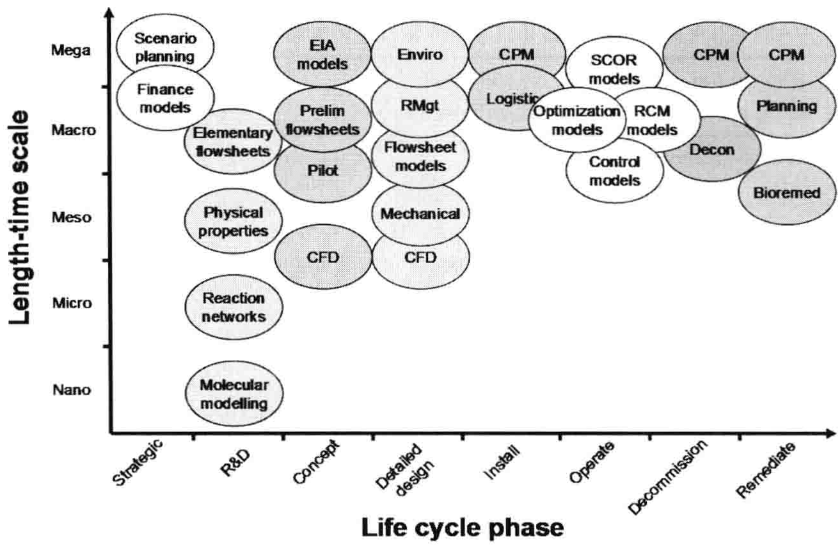

FIGURE 3 **Modelling across the life cycle and scale domains.**

Figure 3, which gives a selection of model applications across the product-process life cycle, emphasising not only the individual life cycle phases, but also the relevant scales of the system being addressed. This emphasises the multi-scale, multi-form nature of current modelling practice.

What becomes evident from Figure 3 is the very wide spread nature of product and process modelling, across all life cycle phases. Scenario planning and economic assessment models are used for long term strategic planning of companies and organizations. Research and development employs a wide range of models, potentially applied to understanding the fundamental aspects of the products, their properties and the processes that will produce them. In conceptual and detailed design, many decisions are informed through model use, whilst the rest of the life cycle phases use numerous models, for decision making purposes.

A major development over the last 20 years has been the ever increasing scale expansion, whereby modelling is addressing quantum and nanoscales, to mega or global scale issues related to supply chains and global climate variability. It is now a 'model-centric' world of product and process engineering. Table 2 gives a summary of the life cycle phases, some model applications, forms and approaches.

Figure 3 also shows the scale focus of concern, often associated with specific life cycle phases. Some phases are focussed on large-scale issues, whereas other phases reach deep into the lower scales, to resolve uncertainties that might be