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AN INTRODUCTION TO MODELS

1.1 What this book is about and why it was written

A cheese paté bitten in mistake for a sweetmeat is likely to produce revulsion whatever the quality of the cheese and so, as this book is an unusual confection, it may be as well to give the reader at the outset some idea of its ingredients and why it has been thought worthwhile taking the trouble to concoct it.

Briefly, we have attempted to provide an introduction to modelling in general and a more advanced treatment of some important aspects of the use of models in academic and industrial fields ranging from speculative research to the developing of useful new products. The treatment seeks to bring out themes that are relevant to many of the diverse fields in which a chemist may nowadays be asked to contribute. Additionally, the central chapters of the book that deal with chemistry *per se*, provide a novel revision course for a substantial part of the subject.

The authors, two of whom were working in universities and one in industry, talking together about their work noticed that the discussion frequently turned to models and modelling, and that within these fields there were concepts which fitted together to make a framework in which their very different problems inter-related. The topics that happened to be under discussion at the time were, in the academic camps the use of model compounds in the study of biosynthetic pathways and of biological mechanisms, and on the industrial side the use of mathematical models of processes that were under development and of small-scale (semi-technical) plants as models of proposed manufacturing units. The authors were aware of the use of models in many other activities in which scientists participate and knew that these also would fit into the same framework of ideas.

There is, of course, nothing new in the observation that general concepts exist that are applicable to modelling across a wide area of pure and applied science, or in the recognition that these may be both intellectually stimulating and useful in practice, but though there are many excellent texts that have relevance for one or more aspects of modelling in chemistry, we have found neither a critical review of the practice of modelling in academic chemistry, though much work based on models has been published, nor a review of the principles of modelling as it may be applied over the many fields of activity in which a chemist may be required to practise at some stage in his career.

Passing reference to some important aspects of modelling, to the advantages and to the dangers, are to be found in the chemical literature. For example, Mislow (ref. 1) draws attention to a most important caveat that models should not be used under conditions for which they were not designed. Writing on the use of physical models of molecules he emphasises the fact that molecular models are built to reflect the behaviour of an 'average' molecule at near room temperature and cannot reflect the changes in the properties of molecular aggregates which result from variation in temperature. But, despite scattered allusions to some important aspects of modelling, there appears to be no general review.

On the other hand, one may discover equally readily papers that demonstrate the need for a clearer appreciation of modelling. The following quotation from a paper on flavin dependent oxido-reduction (ref. 2) while making, at least implicitly, some important points affecting the use of models, for example the need to relate them to their environment, suggests some difficulty in handling concepts in modelling.

> Models should not be any longer conceived as 'homunculi' or as 'bigger elephants than nature' or as micromolecular substitutes for macromolecular catalysts, but simply as derivatives of a coenzyme or a prosthetic group or even a mere protein functional group, which help in understanding the activation of the cofactor by the protein in terms of molecular structure.

But every vacant niche in the literature is not necessarily ripe for colonisation however attractive it may seem to potential authors. We would not have set to work on this book had we not believed that chemists who cannot use models effectively are likely to be seriously disadvantaged in the wider use of their skills.

The principal role of chemistry, it is often argued, is increasingly

Cambridge University Press
978-0-521-29932-9 - Chemistry Through Models: Concepts and Applications of Modelling in Chemical Science, Technology and Industry
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that of an enabling science. Certainly in the academic field the chemist's work overlaps more and more that of other disciplines, whoever may be said to take the lead. Beyond the university, chemists are applying themselves to an ever greater extent to tasks, often interdisciplinary, that lie outside the ambit of their own expertise. All this inevitably creates a need for chemists who can understand and interact effectively with practitioners of other disciplines, among whom must be included economists and sociologists. Indeed the increasing expectation that scientists will accept a share of the responsibility for the consequences of their work demands still wider skills, skills related to those of the designer.

Traditionally however the chemist has not been trained to cope with these requirements. Chemistry (like anatomy?) tempts its disciples to the relatively unstructured accumulation of facts. In academic courses, introductions to other disciplines are often introductions to facts rather than to underlying patterns of thought, which is to say to models. We are, of course, well aware of the great advances that have been made in teaching, in many centres, over the last decade or so; advances to which we hope our own presentation will prove to be complementary.

The scientist's social responsibility is, in large part though not totally, that of ensuring that the artifacts that he helps to create are not at odds with their working environment but rather that they are a good fit. The failures of the past have often occurred through concentrating on immediate technical problems to the exclusion of other factors. Too often the scientist perceives his contribution solely in terms of discovery or invention and fails to recognise that the translation of a new capability into practice – that is to say the process of innovation – requires or imposes changes in people's behaviour, changes that may offer opportunities to some, but for others impose constraints. The avoidance of mismatch between the products of innovation and their task environment is a problem of design, and the process of design employs models in many ways that extend from defining the task to testing the solutions.

One objective of this book is to suggest that inter-disciplinary interaction is most likely to be effective when it is based on an understanding of the conceptual models that the various disciplines use, rather than on mere learning of data, and also that useful models may be found in very unexpected places. In the hope of demonstrating this latter point we have not hesitated to quote rather than to paraphrase whenever we have felt that by doing so we can provide a direct contact with other people's models in a relevant context.

Much of this book is very relevant to disciplines other than chemistry and indeed to other industries, and examples are drawn from several areas, not only from those chemical. However, the unusual combination of topics that we present, though absolutely essential to the development of the theme we have chosen, undoubtedly creates difficulties. Some of these, for example the need for a cohesive treatment across all the chapters, are either met by the authors or not at all, but for others we must ask the indulgence of our readers. Those accustomed to modelling or, indeed, who are specialists in particular fields, may feel an unevenness in depth of treatment across the subject matter. This reflects partly the interest of the authors, but mainly the fact that for some of the topics with which we deal, for example process development, there is already an extensive literature compared with which the contribution in this book must be relatively light. On the other hand, though there are many published examples of modelling in biochemical synthesis, there is little in the way of analysis of its conceptual basis or its relationship to modelling in other fields. On this topic, therefore, our contribution breaks more new ground. Some of those who were good enough to read chapters in draft have suggested that the use of modelling in synthetic, degradative, and biological chemistry, and also in the discovery and development of new products, deserve books to themselves. If this be so, then perhaps the limited treatment that we have been able to give will serve as a stimulus for more extended studies.

It has also been suggested that since we cannot avoid trespassing, however reluctantly, on the preserves of the historians and philosophers of science, we should tramp these fields more boldly. But this is frankly not our purpose nor within our competence, though we do hope to encourage some readers who might not otherwise do so to explore these subjects for themselves. A beginning might be made with Mary B. Hesse's *Models and Analogies in Science* (ref. 3) in which a number of concepts that are of value in practical modelling are advanced during an exploration of the question of whether a theory must logically contain models and analogies if it is to be predictive and therefore accepted as scientific.

Modelling, like all techniques, can be a springboard or a strait-jacket, creative or constricting. Moreover, the more powerful the tool the greater the damage when it is misused: the more fascinating the technique the more serious the risk of addiction. Our experience makes us all too alive to these possibilities and we take care to point out pitfalls insofar as we have been able to perceive them (chapter 2.7).

1.2 What is a model?

Modelling as considered in this book consists in constructing alternative, usually simpler forms of objects or concepts, in the expectation that the study of the model will shed light on the nature of those objects or concepts.

We need a name for that which is modelled and we shall use 'prototype' for this purpose. The *Shorter Oxford Dictionary* defines prototype as: 'the first or primary type of anything: a pattern, model, standard, exemplar, archetype'. Our use of prototype may slightly expand this connotation but there is at least one precedent in the publications of the Delft Hydraulics Laboratory. (Models are, of course, extensively used in investigating hydraulic problems, for example in studying the effects of tides and rivers on land conformation as well as in ship design. The Delft publications provide much useful commentary of general relevance to modelling, some of which we will mention in a later chapter.)

We will not use the word 'model' to connote an archetype or exemplar because, for our purposes, the essence of the model is that it is a restructuring or reformulation – that is to say a model is some transformation or other of its prototype.

It follows that a replica, in the sense of an exact copy, is not a model in our sense of word. Of course, what constitutes an 'exact copy' – a replica – depends on the depth and extent of the comparison. In a later chapter we refer to a radioactively labelled molecule as a model. It has been put to us that this is not a model of the unlabelled compound but a replica. If no radioactive effect were expected or sought then 'replica' might be an appropriate description – unless the label produced some other change that was significant for the purpose in hand. But this may well be the case. Isotope effects on reaction rates are common. As is well known, C–D and C–T bonds break roughly 7 and 14 times slower respectively than C–H. ^{12}C–^{14}C breaks in many reactions about 10% more slowly than ^{12}C–^{12}C and since ^{14}C may be present at a level of only 0.1%, this may have a significant effect on where and when to look for labelled products.

These are more recondite examples of differences in behaviour between labelled and unlabelled molecules that, being most unexpected, emphasise the need for constant care. One example must suffice. Some terpenes can be separated by differential absorbtion on a column that is composed of silica gel impregnated with silver nitrate, in which the C–C double bonds complex with the silver cations. In some instances when this technique has been used with terpenes labelled with tritium, the tritiated compound has been separated from the unlabelled molecules on the column. Failure to spot this could clearly have led to erroneous conclusions.

It is always safer, in experiment and in design, to think in terms of models rather than of replicas, and therefore to expect the unexpected discrepancy. Replica is a courtesy title that events may revoke at any time.

The identification of 'model' with 'prototype' as something to serve as a standard or to be copied is common usage. Kuhn uses the word in this sense when discussing those networks of scientific achievement that scientific communities acknowledge as providing, for the time being, the foundations for its further practice and which he has called paradigms: he writes (ref. 4)

> Achievements that share these two characteristics... (attracting an enduring group of adherents away from competing modes of scientific activity and being sufficiently open-ended to leave all sorts of problems to be solved)... I shall henceforth refer to as 'paradigms'... By choosing it (paradigm), I mean to suggest that some accepted examples of actual scientific practice – examples which include law, theory, application and instrumentation together provide models from which spring particular coherent traditions of scientific research.

Kuhn's paradigms are models in our sense also.

The different meanings of 'model' though potentially confusing should not cause difficulty as they are readily distinguishable. It is advisable, however, whenever the term model is encountered, to check from the context what is intended.

To talk of 'a model of a prototype' is not necessarily to imply that the prototype exists. A model may be constructed before its prototype as a partial realisation of something that one may wish to create. A map of a stretch of countryside is obviously a model of an existing prototype but, on the other hand, the ground plan of a proposed motorway is a model of a prototype that exists as yet only as an unrealised concept. The model is, in such cases, a tool to be used by the design team both to test the appropriateness of their plans and to assist in translating the final design into actuality.

Often, in the process of design, a series of models will be constructed each of which is intended to provide information on a particular aspect of the behaviour of the prototype. Sometimes the models will, as it were, converge on the prototype so that eventually one is accepted as defining and expressing for the time being *the* prototype, a standard and to be copied – as in the aircraft industry. Much of the expense of aircraft development arises from the fact that the reliability of so complex a system, consisting of thousands of interacting parts, cannot be confidently predicted from the behaviour of models each of which necessarily suppresses some interactions that may prove to be operationally important. As a result, extensive testing has to be done at full scale and with the entire aircraft. Likewise in the design of chemical plant it is sometimes necessary to undertake tests at full scale, though the overall problem is less because it is usually easier to provide protection against the consequences of component failure.

1.3 **Types of model**

Depending on the purpose in view one can define many different types of model and classify in various ways. A useful categorisation of models and a formal analysis of their taxonomy and development will be found in Mihram's paper *The Modelling Process* (ref. 5).

For the purpose of this introductory chapter it will be sufficient to classify models broadly as physical or conceptual, the latter including mathematical models. That models of these types are fundamental to learning – in organising ideas in such a way as to be able to predict effectively from experience – is very clearly explained in Bruner's *Towards a Theory of Instruction* (ref. 6) which book, incidentally, we would strongly recommend to anyone who is interested in inter-personal relationships (and who should not be?).

To go beyond the responding to information encountered on a single occasion and to predict the future on the basis of experience, the individual must store information in some structured way that corresponds to his environment. Bruner considers this to be the essential process of learning and suggests that the child develops three types of model.

Cambridge University Press
978-0-521-29932-9 - Chemistry Through Models: Concepts and Applications of Modelling in Chemical Science, Technology and Industry
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The first way in which the individual can translate his experience into a model of the world is, Bruner suggests, through action.

> We know many things for which we have no imagery and no words, and they are very hard to teach to anybody by the use of either words, or diagrams and pictures. If you have tried to coach somebody at tennis or ski-ing or to teach a child to ride a bike, you would have been struck by the wordlessness and the diagrammatic impotence of the teaching process. [Ref. 6*a*.]

This type of modelling Bruner calls enactive, and we can see a close parallel in the behaviour of those scientists and engineers who like to begin tackling a problem by experiment, by doing something with their hands, by twiddling the knobs.

Bruner's second system is based on summarising images and he calls it iconic. Some models are, in one way or another, physical representations of their prototype. Examples are: the small-scale plant (often called semi-technical or pilot plant) that is built to provide data for the design of full-scale manufacturing plant, molecular models, maps (including for example plots of electron density and of X-ray diffraction data), and model compounds used in synthetic, degradative and biological studies. It is this kind of model that is called iconic and which Ackoff (ref. 7) defines as follows:

> Iconic models are large or small scale representations of states, objects, or events. Because they represent the relevant properties of the real thing by those properties themselves, with only a transformation in scale, iconic models *look like* what they represent. For example, road maps and aerial photographs represent distances between and relative positions of places and routes between them. With respect to these relevant properties such maps or photographs look like the real thing: they differ from it with respect to these properties only in scale. Flow charts which show the processing of material or information may also be iconic models, as may be floor plans or other types of diagram.

This definition gives an indication of the difficulty in attempting a logical and consistent classification of models. How, for example, could one define 'look like' to permit it to cover all examples given in the quotation: and does a flow chart differ from its prototype only in respect of scale?

The third type of model, the symbolic or conceptual, is essentially a mental construct that may range from the simply descriptive to the rigorously analytical and in which the symbolism may be as varied and loosely defined as a pattern of thought or as precisely defined as an algebraic equation. Like other types of model, symbolic models may be static or steady-state models or they may be dynamic and represent changes that occur with the passage of time.

Scientists are often dissatisfied with models that are not developed beyond the descriptive stage since at that level no quantification and therefore no rigorous experimental testing is possible. Nevertheless, much that is vital in modelling takes place at the descriptive stage. Experienced workers will agree that more models fail to be useful, or even positively mislead because they are inappropriate than fail through neglect of rigour or through inadequacy in mathematical techniques. If we fail to ensure that our model is relevant to the problem in hand, that significant characteristics of the prototype and of its relationship to its working environment have not been overlooked, then no degree of sophistication in its representation or manipulation can remedy the deficiency. It is at the descriptive stage that most decisions on these important matters are taken and it follows that a good descriptive model may, indeed should, present a useful analysis of the factors that are significant in the situation under study.

Perhaps the most important of his conceptual models is each person's private representation of the world about him. Beer, in his book *Decision and Control* (ref. 8) which is strongly recommended as provocative, stimulating and useful (as is also his latest book *Platform for Change* (ref. 9)) writes

> Rational conduct depends not only upon knowing what is really happening and being able to interpret it, but on having present in our minds a *representation* of what is going to happen next. This representation is not an account of what is the case, but a continuous prognosis of what is about to be reported to us as being the case. It is a prognosis continuously corrected by the feedback. Let us call this mental representation of the world that is not a direct perception of the world a model of the world.

This model is, of course, not fully verbalised, indeed it may not be entirely at the conscious level. It is a dynamic model that predicts the behaviour of the real world. Expectations are compared with what actually happens and the model is continuously updated to eliminate discrepancies.

In the absence of feedback, as seems to be the case in dreaming, bizarre results may ensue. In the waking state, when apparently important messages reach the consciousness – or perhaps before – we attempt to verify them. On hearing the fire alarm we look for flames or smoke and sniff the air. The result of these investigations constitutes an element of feedback into the system. In that state of sleep in which intense dreams occur we are unable to interrogate the environment and are deprived of recourse to our enactive models. All but the most intense external stimuli are shut out. The patterns of which we are conscious, though they may be entirely unrelated to the current state of the real world or, sometimes, an attempted rationalisation of one intense stimulus (ref. 10) are accepted as a model of it and may stimulate emotion as intense as that which we experience when awake. Dream experiences, at least frame by frame, may be heavily transformed models of past experience but the correspondences are often difficult to identify.

Bruner sums up his thinking on the three types of model thus (ref. 6*b*)

> What comes out of this picture is a view of human beings who have developed three parallel systems for processing information and representing it – one through manipulation and action, one through perceptual organisation and imagery, and one through symbolic apparatus. It's not that these are 'stages' in any sense; they are rather emphasis in development. You must get the perceptual field organised around your own person as centre before you can impose other, less egocentric axes upon it, for example. In the end, a mature organism seems to have gone through a process of elaborating three systems of skill that correspond to the three major tool systems to which he must link himself for full expression of his capacities, tools for the hand, for the distance receptors, and for the process of reflection.

We have quoted Bruner at some length not merely because he provides a concise and elegant psychological basis for the two major categories of model: iconic, and symbolic or conceptual, and in his enactive model for the practical scientist's often irresistible temptation