MODELLING as RESEARCH METHODOLOGY

Revised edition

G.D. Jordaan & L.O.K. Lategan

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(Editors)

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PREFACE

There are a few research methodologies that can be used in all disciplines and sciences, both natural and human. Modelling – both scale and mathematical modelling – is an example of this important, universal commonality in research.

To study a small segment of a large natural phenomenon in a controlled manner is typical of research in natural sciences. Hence, for practical reasons, a representative model of the actual phenomenon is studied rather than the complete phenomenon *per se*. Results obtained from such can then be extrapolated so as to enable a better understanding of the phenomenon and its expected behaviour under certain conditions.

Alternatively, a mathematical representation of a system can be developed, and its functioning studied indirectly through the solution of the mathematical model for specified conditions. Although this technique is particularly common in engineering-related studies, social and economic matters also lend themselves to this particular methodology through the development of suitable mathematical models that describe the functioning of a system.

Modelling can be utilised in virtually any discipline, and can also fulfil different functions. The most typical use of models is to try and understand or study the (probable) operational characteristics of a physical system under predefined conditions, or to assist with the design and development of a new system, meeting specified operational characteristics.

The increasing complexity of society, together with the devices that it utilises, has resulted in a situation where procedural models are even used to describe the optimal way in which a new system is to be designed, developed, and eventually its functioning assessed.

Especially in engineering-related research, it is common to design, build and assess the functioning of scale models of physical structures and functional units. These techniques facilitate the determination of the expected functioning of the actual structures or systems under investigation.

An important stage in the modelling process is verification of the validity and accuracy of a model. This is often done by accessing measured values on the actual system as developed and built, and comparing them with the modelled values of the same system. A data acquisition system is usually required to access such data and save it in a computer's memory for processing and interrogation.

This book is a modest attempt at introducing the basic principles of modelling and its associated practices, as well as illustrating this research technique by means of a few practical examples of its use in a variety of disciplines. It is hoped that this will contribute to an improved understanding of the underlying principles of (potentially) one of the most important, yet often neglected, research methodologies.

Jorrie Jordaan & Laetus O.K. Lategan
(Editors)

SECTION 1

General Principles of Modelling

CHAPTER 1

Principles of Modelling in Research and Design

Gerrit Jordaan

1. MODELLING

The principles of modelling, within the context of this book, involve several categories of systems of representation of a functional system or phenomenon. In particular, mathematical and physical (e.g. scale modelling) of prototypes (the planned, final product, structure or phenomenon under consideration) are important research practices in both natural and human sciences.

Modelling is also often referred to as simulation, where it describes the representation of an actual situation by a mathematical model, or alternatively by laboratory apparatus in the case of a physical model [3]. The term "modelling" is also used to describe the practice of functionally dividing an operational unit into a number of different sub-units, the operational parameters of each of which can be defined as an element of the whole unit.

Even though modelling inevitably facilitates a better understanding of the expected functional characteristics and limitations of a real-life system, many researchers still do not use these research techniques optimally in the study of phenomena that could be modelled successfully. For a long period, there was a tendency to use mathematical modelling predominantly for the study of engineering-related problems. Fortunately, this is no longer the case, and it is increasingly being used to model phenomena that occur in other natural science disciplines, as well as in the human and economic sciences.

2. MATHEMATICAL MODELLING

Mathematical modelling is the process of describing the behaviour of an element of a physical system, or a comprehensive system or phenomenon, by means of a mathematical expression, or a series of mathematical expressions. This can only be done after the identification, definition and quantification of the interrelationship of those variables with a substantial effect on the functioning of the system to be modelled. Thus, the effects of these variables on the performance of the system should be determined and represented mathematically to enable mathematical modelling of the system.

Figure 1.1 is a representation of the practice of modelling, indicating the process of:

- construction of a model of a phenomenon that occurs in the real world and needs to be studied;
- using mathematical theory to analyse the model; and
- acquiring results of the analysis and interpretation thereof in order to interpret the phenomenon that is being studied.

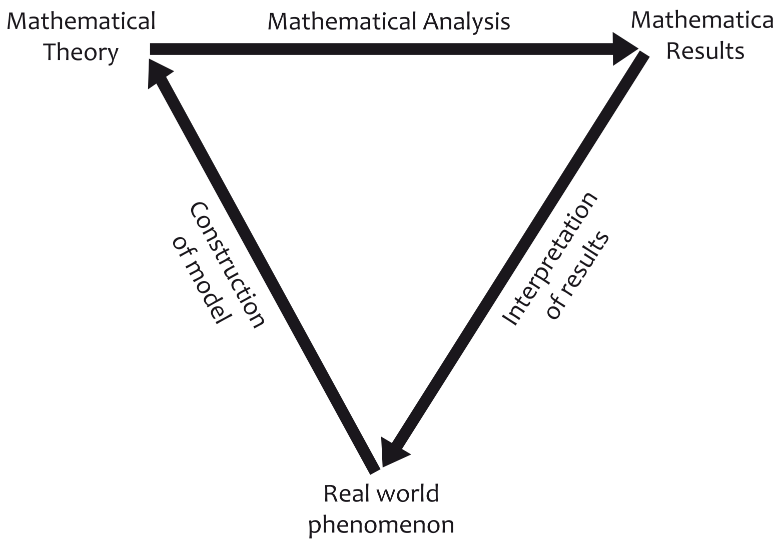

Figure 1.1: The principles of mathematical modelling

A system is usually a set of interacting and/or independent elements, real or abstract, forming an integrated whole and functioning collaboratively and interdependently. The functioning of the system under specified conditions depends on the characteristics of each of its constituent elements. It is common to identify and describe the different elements of a system and to express the operation of each mathematically. By sequentially varying the values of one input variable between predetermined limits, whilst monitoring the effect of this on the functioning of the complete system (the output), it is possible to investigate the effect of the particular input condition on the functioning of the system. In this way, a better understanding of the different elements, and its expected effect on the functioning of the complete system, is developed.

With reference to Table 1.1, an outcome of this type of simulation could be a graphical representation of the output power of a wind generator with an increase in wind speed from, say, 10 to 50 kilometres per hour.

Figure 1.2(a) below shows a particularly accurate simulated response of an electric motor under certain, specified input conditions [5]. It depicts the expected (predicted) speed and torque of the motor under certain conditions, whilst Figure 1.2(b) shows a set of measured values for the motor when it was actually exposed to the same input conditions [5]. From this, it is evident that the mathematical model of the expected torque and speed characteristics of the motor was such that the characteristics of the motor could be predicted very accurately.

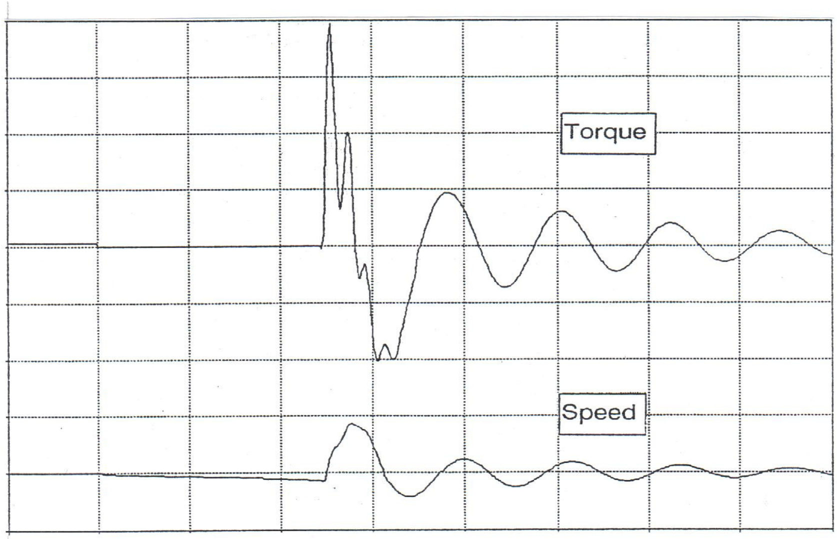

Figure 1.2(a): Simulated functioning of an electric induction motor under specified conditions

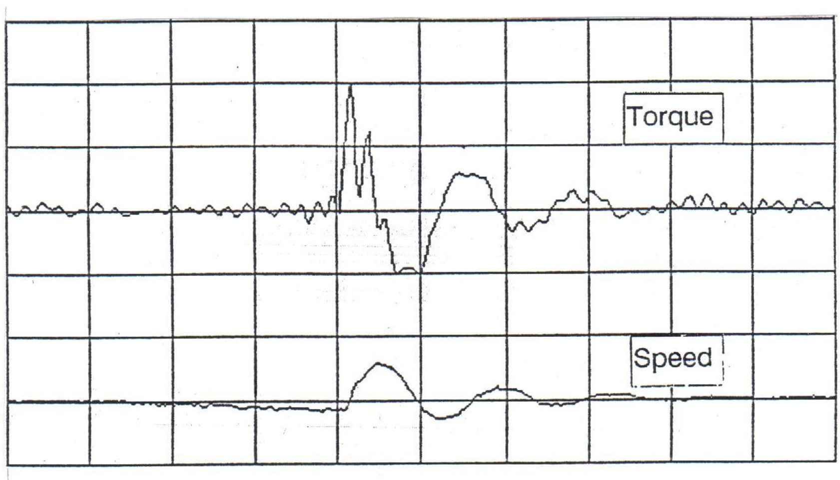

Figure 1.2(b): Measured performance of the simulated induction motor under the same specified conditions

Careful inspection of Figure 1.2(b) reveals substantial electrical noise on the measured characteristic. This does not necessarily detract from the validity of the simulation, but illustrates the need for experience and background knowledge on the part of the researcher for the accurate assessment of such results.

To facilitate easier modelling of a problem, the system is often simplified by limiting the number of variables modelled to those most critical to a description of the functioning of the system. Obviously this can only be done if there is a thorough understanding of the underlying functional principles of the system, otherwise variables critical to the functioning of the system may be ignored with a consequent fatal decrease in the accuracy of the developed model. In this way, very complex systems can be described and studied as combinations of relatively uncomplicated, understandable subsystems (elements) – for each of which there is an approximate analytical solution available.

With increasing evidence that an accurate model successfully describes the behaviour of a modelled system, the confidence of the modeller in his model will increase and it will usually be used increasingly.

The modelling of mechatronic systems, including a combination of both electronic and mechanical parts, dynamic and static components with hysteretic effects, flip-flops, and sensors, as well as effects like inertia, elasticity and friction – thus a hybrid combination of continuous and discrete state elements - is particularly difficult. This typically necessitates the use of special system formulations [1].

2.1 Availability of analytical solutions

Any system for which an approximate analytical solution for its behaviour is available – or can be derived – can be modelled mathematically and its functioning simulated numerically. This is normally done by considering the system as a combination of interactive elements as referred to in paragraph 2 above. Table 1.1 shows a number of typical examples of physical phenomena that can be modelled successfully.

Table 1.1: Typical phenomena to be modelled

Modelled phenomena	Description of possible modelled characteristics
Prevalence of ailments	The prevalence of a certain ailment in the population of a particular community under specified conditions.
The effect of the population size of certain kinds of game	The effect of an expected change in the number of lions on the presence of a particular kind of antelope in a specified area over a specified period of time.
The flight path of an aircraft	The expected flight path of a specific aircraft with a defined load under a complete loss of power condition.

Modelled phenomena	Description of possible modelled characteristics
The functioning of physical structures with varying loads	▪ The behaviour of a bridge under different conditions of dynamic loading. ▪ The effect of an increase in wind on the performance of a wind generator.
The growth of a tumour	The effect of certain drugs on the rate of growth of a tumour.
The operating characteristics of an electrical system	▪ The effect of bandwidth limitations of a transmission line on the recoverability of transmitted signals with specified characteristics. ▪ The expected speed and torque characteristics of an electrical motor under specified electrical supply conditions.
The effect of a particular change in the environment on an insect population	The relative population growth of a certain species of insect if subjected to a specified change in environmental conditions.

The expected behaviour of the system under consideration can be predicted by means of mathematical modelling, whilst the accuracy of the predictions is a function of the correctness of the mathematical formula(e) used to describe the system, as well as that of the boundary conditions and the initial conditions in the case of unsteady or time-dependent phenomena.

It is obvious that mathematical modelling is an extremely useful tool that can be used in a very wide variety of applications, and is only limited by the mathematical abilities and understanding of the modeller of the system under investigation, rather than the discipline in which he or she is working.

2.2 Monte Carlo simulations

In some cases, the modeller would like to determine the effect on the system if several variables should vary simultaneously and independently – normally within a fixed range for each variable. In such a case a so-called Monte Carlo simulation would be executed where the defined set of mathematical expressions are solved repeatedly whilst several relevant variables are adjusted randomly within predefined ranges [2]. In this manner, it would be possible to determine, for example, the sensitivity of a system to possible tolerances of the components used in the construction of the system.

2.3 Simulation software

The programming ability of the modeller, and availability of dedicated simulation software, normally determines the manner in which the modeller would do the actual simulation.

Mathematical simulations are often executed using a standard mathematical software package such as Matlab, Mathcad, Mathematica or Maple. Alternatively, application-specific software with good graphic interfacing or a custom-written programme can be used for this purpose. However, good graphic interfacing is an imperative since the evaluation of a simulation is often easier if the results are provided in a graphical format.

A number of special-purpose computer languages for system simulation have been developed – where the use of any of these languages can eliminate a large amount of effort compared with starting with a general-purpose language such as C^{++}. The General Purpose Simulation System (GPSS) is an example of a specialised simulation language, orientated towards engineering situations and is used for production-flow problems and inventory analysis [2].

A finite element model of a problem gives a piecewise approximation to the governing equations of a structure response. This technique facilitates the detailed modelling of extremely complex shapes [4]. With the recent increase in the availability of good, user-friendly finite element analysis (FEA) software and the exponential growth in the computing power of modern computers, FEA software is increasingly being used to determine the expected dynamic behaviour of complex systems and structures. With this type of software, it is relatively common to accurately determine the expected performance of a complex system at more than, say, a million points of calculation – which, even with today's extremely powerful computers, may take hours of computing to simulate.

3. PHYSICAL MODELLING

Although physical modelling is used predominantly in engineering applications, it can also be used for the execution of controlled experiments in other natural science disciplines.

Aerodynamics plays a vital role in many engineering fields, such as aerospace, architectural, automotive and marine engineering. These phenomena are usually modelled physically in either wind or water tunnels [4].

To some extent, mathematical modelling superseded scale modelling, and facilitates a shorter reaction time in terms of possible changes in the design of a modelled system. However, the use of physical modelling is still very much the order of the day – particularly in terms of the modelling of hydrodynamic and geographical phenomena. In these cases, there is often no analytical solution available and scale modelling is the only viable method to accurately investigate the characteristics of the prototype.

Physical models are often used to visualise a planned construction and can also be used to investigate possible assembly procedures of the eventual product. However, the main application of physical modelling is probably to measure the expected functioning of a system under a specified range of varying (load) conditions. Typical examples of cases where such measurements are made include:

- the effect of an increase in wind speed on the performance of a wind generator;
- the effect of a rise or fall in water level on the deflection of a dam wall;
- the aeronautical characteristics of a system; and
- the vibration of structures due to varying loads.

A physical model of a system typically consists of a scaled down (or in some cases scaled up) version of the complete system, or specific portions thereof. Often the system is simplified by limiting the accuracy to which some, non-critical elements of the system, are modelled. However, a thorough understanding of the underlying functional principles of the system is required to ensure the safe identification of non-critical variables.

As with mathematical simulation, the performance of scale models is often ascertained with one varying variable – such as the functioning of the system over a range of temperatures – whilst the other variables are kept constant. The design of the experimental apparatus and procedure must take into account the preferred degree of automation appropriate for the experiment [3].

4. ADVANTAGES OF MODELLING

The ever-increasing use of mathematical and physical modelling techniques is ample proof of the immense value of these practices for modern day researchers and practicing engineers and technologists. The following examples are indicative of the advantages that normally flow from modelling and simulation in research activities:

- The resultant ease of performing controlled pseudo-experiments.
- The determination of the anticipated effect of any change in the operating conditions of that will influence the functioning of the eventual system – man-made or otherwise.
- Time compression in the sense that a simulated experiment can take a small fraction of time compared to an actual system under test.
- Sensitivity analysis for observation of the behaviour limits of a system.
- Experimentation without requiring the financial outlay for the real system.
- Usually, modelling is an effective training tool.

5. SUMMARY

Modelling involves a repeated switching between the functional and physical characteristics of a system, i.e. the determination of the expected change in the functioning of a physical system if a specific physical characteristic is changed to a certain extent. Or, alternatively, a determination of what would be the required change in the physical characteristics of a system in order to cause a predetermined change in its functioning.

It is frequently required to ascertain the expected performance of a system or structure under development. This would normally be done in one of the following two ways:

- A physical model of the system, with its size normally scaled up or down and with the main physical features that should impact on its performance being prepared in great detail, is built. Its functional characteristics are measured in physical conditions that approach those in which the prototype will be expected to function. From these measured results the expected functioning of the actual prototype is derived or predicted.
- A mathematical model of the system under consideration is developed and its expected functioning is simulated mathematically. From these calculated results, the expected functioning of the actual prototype is derived or predicted.

Either of these methods of investigation can be used, depending on circumstances, to validate a new design or the expected performance of a system. After construction of the prototype it would be normal to validate the accuracy of the modelling that took place by evaluating the performance thereof experimentally. These alternatives are shown schematically in Figure 1.3.

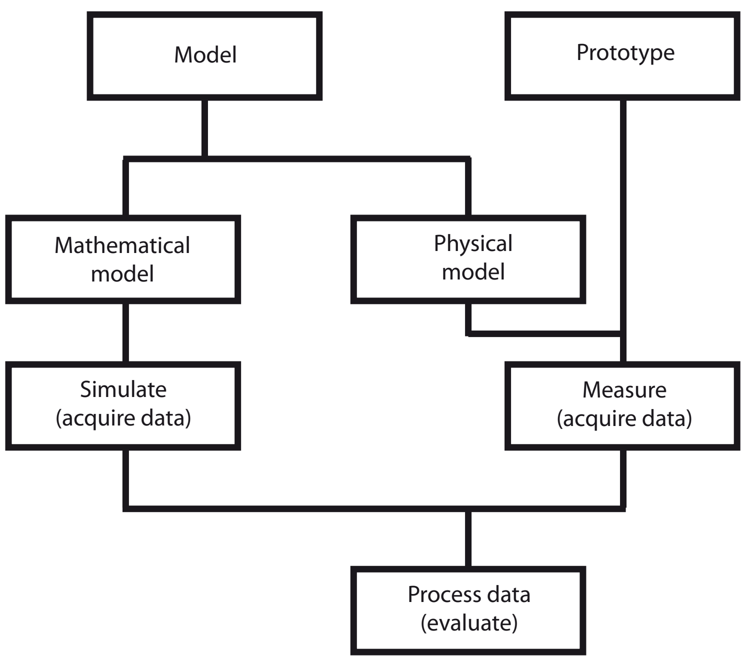

Figure 1.3: Alternative methods to determine the expected functioning of a system or structure under development

Mathematical, physical and functional modelling (and contributions thereof) are well-respected research techniques frequently used by researchers in almost all fields of study to determine the expected performance of a system under development. It is imperative that researchers who are serious about the development and optimisation of new designs should be *au fait* with the relevant principles governing the use of these techniques.

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CHAPTER 2

Models and Modelling for Science

Ulrich D Holzbaur

Science – even applied science – is not concerned with solving individual problems but with describing structures and giving statements in a general setting. To derive a general statement from observations and individual solutions, one needs abstraction and generalisation. This is the essential use of modelling: a model describes only the relevant general aspects and leaves out all individual aspects. In most cases, identifying the relevant and irrelevant aspects and determining adequate models is the most important part of scientific work.

Mathematical models for science are described in this chapter, starting with the fundamental ideas of modelling and a definition of models and systems. To model reality successfully, we have to consider model classification and types from informal to formal mathematical models, the modelling process from the mental model to formal solutions, and from generic models to model instances. Several examples for models in science, especially for dynamic models, are also given.

1. SCIENCE AND KNOWLEDGE

First the relation between science, research and models are clarified. For this, we refer to [2, 3 and 5].

1.1 Knowledge

Research activities are undertaken to gain knowledge. To know something does not mean to own some information, but rather to allow integration of this information into a system of knowledge. For an individual person, this is the cognitive function of the mind.

To represent knowledge within the scientific community, we need some representation of information and knowledge. This representation can be done implicitly, e.g. in the unspoken basics and traditions of culture, or explicitly, e.g. in models with more or less formal syntax and semantics.

1.2 Models and systems

One preliminary remark with respect to the philosophical aspects of modelling is that although models are as real as any part of the "real world", the "real world" concerns those items that exist independently from the envisaged modelling process. As long as modelling itself is not seen as the object of the modelling process, this does not cause any confusion. For the purpose of natural and social science, economy and technology, this differentiation does not cause any paradox and gives a short notation to refer to models as the images, and the "real world" as the pre-image.

- A system is any – real or mental – part of the real world that is identified by considering either the individual parts together with the relations between them, or its boundaries and relevant aspects. A system is often also something abstract since it is not something that can be identified in reality and the consideration of parts of reality is an idealisation in itself.
- A model is a representation of a system that is used for a dedicated purpose. This means that the model itself is a – more or less abstract – system that has some purpose (pragmatics) and some relation to another system (semantics).
- A formal model is a model that obeys some formal rules (syntax) with respect to the components of the modelled system.
- A mathematical system is a mathematical structure (e.g. a set of equations or relations) that can be used as a mathematical model for a class of systems. From a mathematical system, very general results can be obtained – e.g. on the stability of the system – that will be valid for all kinds of models and systems for which this mathematical system is a valid model.
- A mathematical model is a mathematical description that is used as a model for any complete and consistent set of mathematical equations and which corresponds to some entity, its prototype.
- In the theory of logic, the notion of a model is also used for a system that fulfils (makes true) all statements of a system of mathematical axioms. For example, the surface of a sphere is a model for a non-Euclidian geometry in that it fulfils all axioms except the parallel postulate (on a sphere, any two straight lines meet in two points). The existence of a model shows that the system of axioms is not contradictory.

1.3 Example: From optimal control to linear feedback systems

As an example of a set of mathematical systems that can be used as mathematical models, we consider a continuous time dynamic system. The following descriptions are intended as an indication of the variety in abstraction and complexity of mathematical systems and can of course not serve as an introduction to systems and control theory.

In a rather general setting, a dynamic system is ruled by a systems equation [1, 4]. To this, we can add concepts of control, uncertainty, stochastics, optimality or even game theory. The resulting mathematical system could serve as a model of almost any process – from physics to macroeconomics. To allow a mathematical treatment of the model and a self-contained analytical solution, we have to add assumptions, e.g. linearity. One possible model that can be handled analytically is the linear finite dimensional optimal feedback control system that is well known in engineering and economics.

Starting from basic principles on deterministic memory-less dynamic systems, the system is modelled by a state x that evolves in the course of time. The future evolution of the system from some time t_1 depends only on the state x at time t_1. In the formalism of systems theory, the transition law is given by $x(t_2) = T(x(t_1), t_1, t_2)$. Note that finding an adequate state (space) that contains all necessary information is one of the important steps in modelling. For example, to describe the dynamics of a mass point in space, we have to consider the six-dimensional state vector consisting of position and velocity.

The transition function for the controlled system would depend on the values of the control input on the interval $[t_1,t_2]$. We can write this as $x(t_2) = (x(t_1),t_1,t_2,u[t_1;t_2])$. Next, we assume the very special case that the system is linear and governed by a differential equation.

$$\frac{dx}{dt} = Ax \tag{1}$$

where A is a square matrix that describes the system's dynamics. The (uncontrolled) transformation function T is now given by the solution of the differential equation.

$$T(x(t_1),t_1,t_2) = E(x(t_1)t_2 - t_1) \text{ with } E(x,\tau) = e^{A\tau}x \tag{2}$$

The dynamic behaviour of the system, explicit solutions, and stability can be analysed mainly by considering the eigenvalues of the systems matrix A. The linear control system is given by the differential equation.

$$\frac{dx}{dt} = Ax + Bu \,, u = C(x - x_0), \tag{1´}$$

and describes the dynamic control aspects of a vast range of systems from engineering (control of a power plant, speed control, target tracking), economics and management (all types of control), and cybernetic systems in social, natural and life sciences. It describes a very generic system with a huge variety of potential instances. From this mathematical system, we can start to model the real world system.

A mathematical system becomes a model when the variables are given a (general or special) meaning. Hence, we can define generic mathematical models, such as the model of technical control systems, by saying that x is a physical variable; more special models, such as the speed control in a car, by defining x to be the speed of the car; and model instances that describe the cruise control of a special (type of) car considering the dynamics of this car.

To determine the optimal control function or optimal control law, we need a criterion for the quality of the dynamic behaviour. This can be modelled by combining three criteria: the deviation (magnitude) of x over time and at the end of the control period, and the efforts for influencing the system. We could also integrate other criteria and, for example, explicitly consider the time T to reach a state $x = 0$. In the linear-quadratic case, the cost model can be described by:

$$Q = \int_{\tau=0}^{T} x(\tau)' M_S(\tau) x(\tau) + u(\tau)' M_R(\tau) u(\tau) d\tau + x'(T) M_F x(T)$$

Here, the $x'Mx$ are quadratic forms which in the one-dimensional case just give a product x^2M. M weights the states (S) and resources (R) over time and final results (F). Applying the quality criterion to the linear feedback system, we find criteria for the optimal control law u, for the existence of a linear optimal feedback control law $u(t) = C(t) \cdot x(t)$ and for the optimal feedback matrix C.
The time-discrete approach can be used to derive a similar type of optimal control problem. Time-discrete stochastic models with finite state can be modelled via Markovian decision models that can be handled algebraically. Also, these discrete time finite state models can be used for a wide variety of real world problems – such as for optimal resource deployment.

1.4 A model of modelling

The following are very formal considerations on modelling, which show the essentials of model-based reasoning.

A formal model

We can model the model criteria in the following way: The result from an action (analysis, transformation, measurement) in the model must be the model of the result from the action. This can be represented as in Figure 2.1.

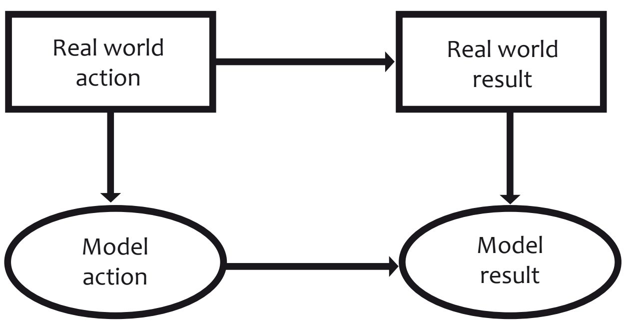

Figure 2.1: Criteria for a valid model

Defining formally the mapping for modelling m and for the effect e of an action, we have $e(m(x)) = m(e(x))$ or $m \circ e = e \circ m$ which means that the diagram commutes. In fact, the mappings for the effects in the real system and in the model are different since they are defined on quite different structures: $m \circ e_R = e_M \circ m$. We also have to take into consideration that neither m nor e_R can be modelled formally.

An example: maps

Let us consider a geographical map as a simple example. A map depicts some part of reality for some purpose. A roadmap should show the road from a place p (city, building) to another place q. For navigation or artillery, we need the direction (bearing) and the distance from p to q. A geological map should show specific subterranean details at a point, say p. Depending on the intended use and the necessary accuracy we have different scales and different projections to allow us to determine these results from the map.

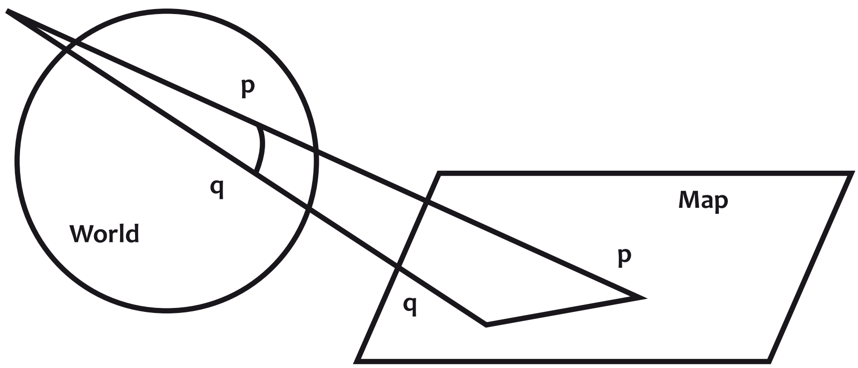

Figure 2.2: Projection as a means of mapping

Several mapping techniques have been developed to model the globe as a two-dimensional map - with most of them being projections. The criterion which we have for the distance d between a pair of points (p,q), would be that $d_M(m(p),m(q))=m(d_G(p,q))$ where d_M and $d_G(p,q)$ are the distances measured on the map and globe respectively while m denotes the mapping (left hand side) with respect to the scale (right hand side). This is possible for larger scales, e.g. on a hiking map, while for larger distances, there is a difference in distance between a flat map and the (approximately) spherical surface of the earth.

The semantics of maps also differ widely with the intended use. For instance, a line may mean a road, a power line, a border, a geographical fault, a contour line or some line of a coordinate grid or search grid. Also, the geographical symbols have some semantics which should be explained by the caption. Depending on the scale, a lot of abstraction and generalisation is used in maps.

A model view on measurement

As seen in the example on maps, measurement is a special case of an action for which models can be used. A model should provide the result of a measurement by manipulation within the model.

The simplest model of measurement is that of comparison: To measure a length in space or in time, you compare the object to be measured with a standard scale. More complex measurement involves the concept of inverse mapping and stochastics:

Let x be the phenomenon we want to describe and e an experiment with outcome $e(x)$. Then we can describe the relation between modelling and measurement as follows:

The effect e should fulfil the following requirements:

- The value $e(x)$ can be measured more easily;
- The relation between x and e is given by a model.

To measure x, means to perform several experiments and to determine the outcomes $e(x)$ and from that to estimate the "best" value for x.

2. USE OF MODELS IN SCIENCE

Due to the benefits that result from the utilisation of models, there is a huge amount of literature about models and (examples of) modelling.

2.1 Models in the knowledge process

In science, we can identify tasks that may be more concrete (based on examples) or more abstract (indicating the integration of knowledge). Models are used in inductive reasoning (from special cases to the general law) as well as in deduction (from the general law to the individual case).

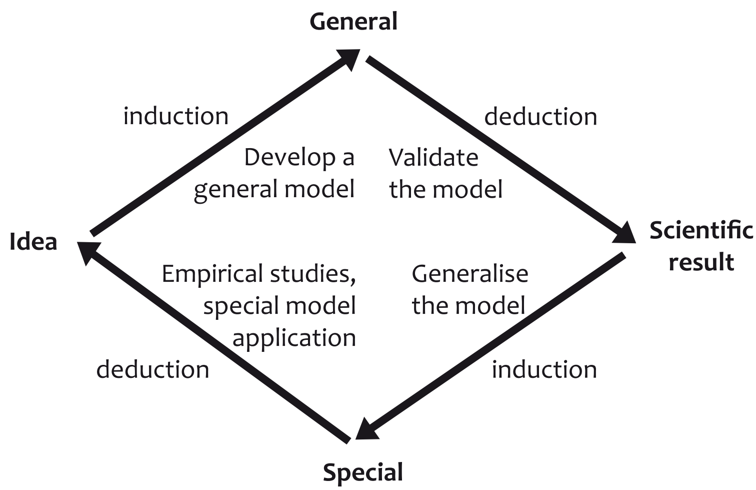

Figure 2.3: Induction and deduction in the knowledge process

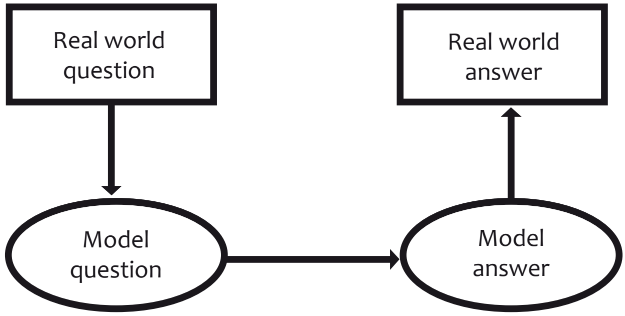

Figure 2.4: Deductive reasoning

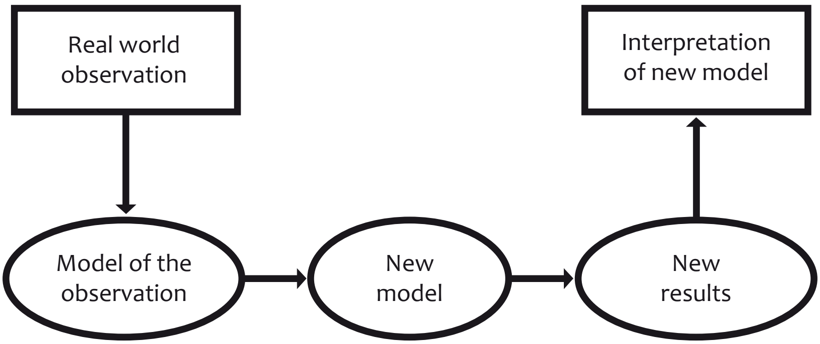

Figure 2.5: Inductive reasoning

2.2 Models in the research cycle

The research cycle begins and ends with the research problem, where the research hypothesis is formulated in an abstract setting and within the relevant discipline. Hence, it uses the notions and notations of the relevant discipline. The research strategy and the analysis and interpretation of collected data link the model-based hypothesis to the real world.

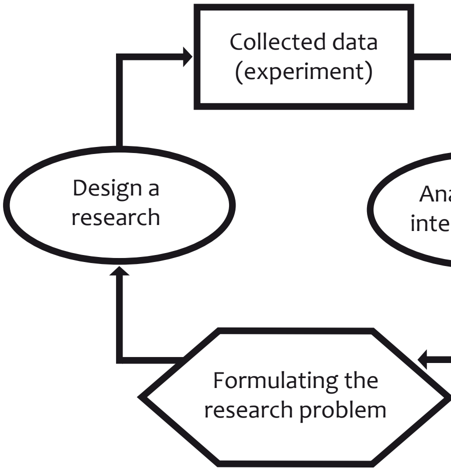

Figure 2.6: Models in the research cycle

2.3 Model-based problem solving

The paradigm of applied science can be described as starting from (possibly, collections of) individual problems, describing structures and giving statements in a general setting. From the models derived, other problems can be solved.

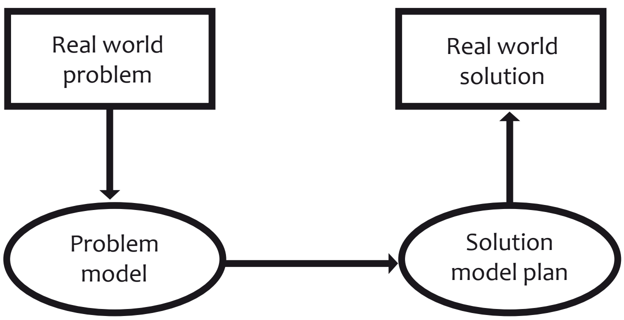

Figure 2.7: Model-based problem solving

Problem-solving methods can be:

- *Mathematical solutions*: From the equations that describe the problem, a mathematical solution can be derived either in the form of another mathematical equation (e.g. the equation of motion (equation 2) as a solution to the differential equation (equation 1)) or as an algorithm (e.g. the Simplex Algorithm on Linear Programming).
- *Computer solutions, especially simulations*: for a discrete time finite state deterministic dynamic system: In principle, the transition function can be implemented on the computer and a simulation can be run. For other system

models, and for a lot of static problems (e.g. FEM), the problem has to be re-modelled.

- *Reasoning, communication and discussions*: Qualitative results and improved insight by using more or less formal models that can be shared among the problem-solving team. This also relates to the motto of "modelling for insight not numbers". Of course, formal solutions and simulations can and should be the basis for this.

3. TYPES OF MODELS

One of the most important steps in modelling – although very often discarded and done implicitly – is the selection of the model type. If you only know one type of model, it is easy ("for a man who has a hammer, everything looks like a nail") and problems are adjusted to the available models like the travellers by Procrustes in Greek mythology.

3.1 Model criteria

The following is an overview of the criteria that can be applied to models and the resulting model classes.

Level of abstraction

In the course of modelling, we go from informal models to more formal models. It is also possible to adapt general models to our individual problem. The different levels of models can be described by three aspects:

- *Abstraction*: How abstract are the objects and relations?
- *Formalisation*: How exact are the semiotics of the model definition (syntax and semantics)?
- *Generalisation*: For how many real life situations can the model be used?

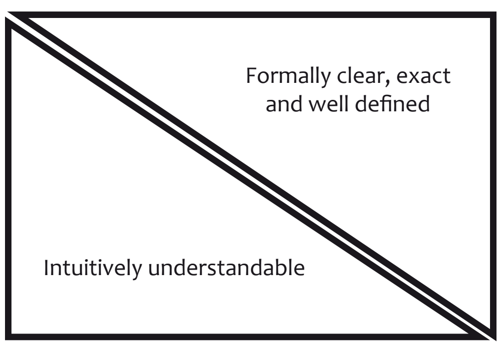

Figure 2.8: Trade-off in model classes

With respect to abstraction, we can consider several model classes with several means of defining the meaning (semantics) of the model:

- Analogue model and scale models;
- Iconic models and pre-models: intuitively;
- Abstract-symbolic models, especially formal models.

The semantics can be defined by intuitive analogy or by formal model semantics. Differentiating material and immaterial models go with the question of whether the content and meaning of the model depends on the materials which the model is made of.

- Material models, which can be classified according to the materials used. These are physical objects such as scale models, analogue models or symbolic-iconic models.
- Immaterial models are independent from the materials they are made of (this may be paper or some electronic representation). They are not defined by the media but by formalism and can be informal models such as texts or graphics, or formal models – especially models from mathematics and logic.

3.2 Model focus and structure

The focus of a model describes the aspects (system-oriented) and perspectives (user-oriented) that are considered within the model. The main focus of a model can be:

- *Behaviour*: input-output-models, black box models;
- *State and event-oriented*: dynamic models;
- *Structure-oriented*: hierarchical models, mechanical models;
- *Flow-oriented*: mechanical flow models, information flow diagrams.

With respect to structure, a model can be flat or can consist of a hierarchy of models.

3.3 Representation of Time

With respect to time, we discern between static and dynamic models. A dynamic model can be just descriptive (kinematic) or can model the causes of changes (law of motion). In the latter case, we usually have a short-term description (law of motion) and a long-term description (trajectory).

Like any other quantity, time can be modelled to be discrete (steps, events) or continuous. While continuous time is modelled via real numbers, discrete time can be modelled via integers (counting the steps) or real number in the case of discrete events that occur in continuous time.

3.4 Representation of Uncertainty

Uncertainty is inherent in any system – from the influences of quantum mechanics to the unpredictability of human behaviour. Uncertainty can be modelled in different ways:

- *Deterministic*: By ignoring uncertainty and replacing uncertain values by "certainty equivalents".
- *Stochastic*: By using the well-elaborated theory of probability to describe uncertainty.
- *Fuzzy*: Using linguistic variables and similar concepts to define uncertainty.

3.5 Representation of Numbers and Quantities

Numbers and quantities can be modelled to be either discrete or continuous. This applies to variables such as:

- Time, duration, events (even discrete events can be modelled using continuous time).
- Space, distances, size, movement, speed (although the concept of speed requires continuity).
- States, properties, flows etc.
- Numbers of objects: Especially huge amounts of individual objects (e.g. atoms, products, people, and creatures) can be approximately modelled by using a continuous model and the set of real-valued numbers. This enables the use of calculus and statistics.

3.6 Usage and pragmatics

The utilisation of a model is the most important aspect since it is the reason for modelling and a criterion for the model to be a model. The usage of the model influences all other aspects. Some important model classes, according to the (intended) type of use, are:

- Descriptive models
- Causal models
- Forecasting models
- Decision models
- Optimisation models
- Normative models

4. EXAMPLES OF MODEL CLASSES

To show the variety of models and model use, two examples for model use in various areas of science are given.

4.1 Flow models

Flows are modelled by network graphs. There is a wide variety of flow models, not only for matter or energy, but also for people, information, money, and value. Though using the same formalism, flows must be clearly discerned from transition diagrams or dynamic systems models. Some important aspects of (static or stationary) flow models are:

- *Magnitude and dimension*: What do the numbers mean?
- *Temporal issues*: Which time (point in time), and duration (interval), is used as a reference?
- *Consistency and conservation*: In flows, we often have a law of conservation (not for information) or consistency requirements for different hierarchical levels.

Example: The global water flow

The following flow model tries to describe the total flow of water on earth. We use it as a basis to illustrate model criteria.

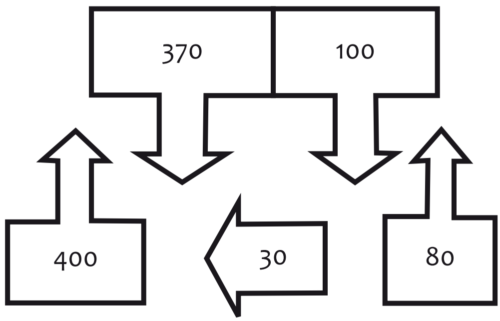

Figure 2.9: Representation of global water flow

To make this model useable, several pieces of information must be added:

- *Magnitude and dimension*: What do the numbers mean? In the example, the numbers refer to the water flows measured in volume per time. The right scale can be calculated from a gross estimate for the earth surface of 40 000 km times 10 000 km, and an annual rainfall of 1 m. From this, a total of 400 000 km^3 or 400 000 000 000 000 m^3 is estimated for the annual rainfall. Hence, the numbers above stand for 10^{12} m^3/Y or 1000 km^3/Y.
- *Meaning*: The two numbers in the upper row stand for the atmosphere; the two lower ones for the earth's surface. The rainfall and evaporation from/to land is shown on the right and from/to ocean on the left of Figure 2.9. The arrow in the middle of the lower row indicates the runoff from land to sea.
- *Consistency*: the conservation of matter is not adhered to: we have a total precipitation of 470 compared to an evaporation of 480. Smaller deviations can be due to rounding (e.g. if the numbers were given in 10^{14} m^3/Y) or measuring

errors, but this difference is not acceptable. This problem typically occurs when multiple sources, measurements and truncations are involved.

- *Display*: As the numbers do not refer to a status but to a flow, they should be displayed by means of arrows. As the last digit is not significant, it should be truncated by using 10 000 km³/Y as a scale.

Considering the lack of consistency above, Figure 2.10 appears to be a more accurate representation of global water flow.

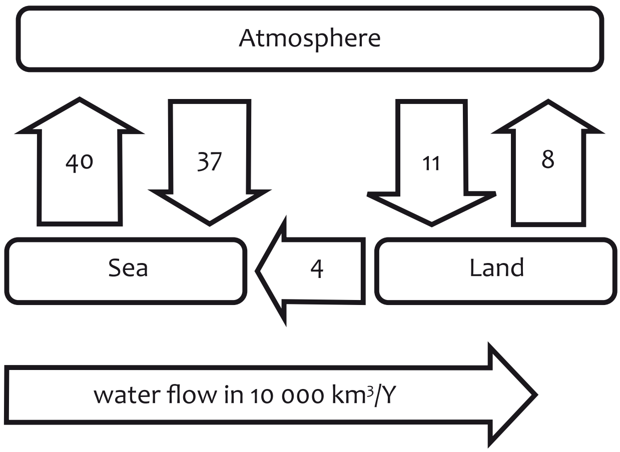

Figure 2.10: Water flow in the global system

Example: Energy flows

As a second example, we consider the analysis of energy flow in a region. With an informal discussion and even balances, we have the problem of properly accounting for feedback loops and heat. Hence, long before we measure flows, we have to clarify what the most important flows are, and where the boundaries of measurement are. The following chart is incomplete but it shows different levels from area to primary and secondary energy to the benefit taken from that benefit. With that basis, we can not only determine the energy flows but also analyse the optimisation of the system (e.g. using surplus heat from combined heat and power-plants to improve the energy efficiency of wet biomaterial) and the impacts of efficiency and sufficiency on the system.

When analysing the material flows of biomass and energy carriers and the energy flows generated from them, circular flows and different levels of energy must be considered. A flow chart helps to keep track of all flows and loops, and makes sure that any summary is done in a consistent manner.

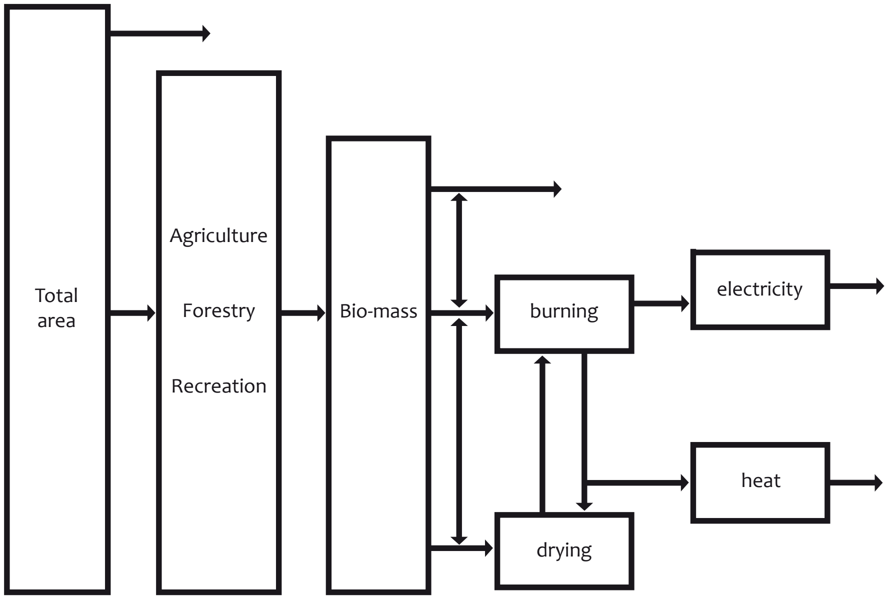

Figure 2.11: A small section of the overall system, modelling the transformation from area to energy flow to human benefit

4.2 Dynamic models

Dynamic models have already been considered in the discussion about mathematical systems. Here we concentrate on the relation between models and solutions.

A kinematic model describes the temporal behaviour of a system, whilst a dynamic model describes the behaviour of a system by means of the laws of motion. Here we have to go from a local description to a global solution.

$\frac{dx}{dt} = f(x,t)$ is equivalent to the integral equation $x(t) = {}^{t}\int f(u(\tau),\tau)d\tau$

This way of describing the dynamics also allows consideration of stochastic differential equations, whilst a second approach is given by a discrete time model.

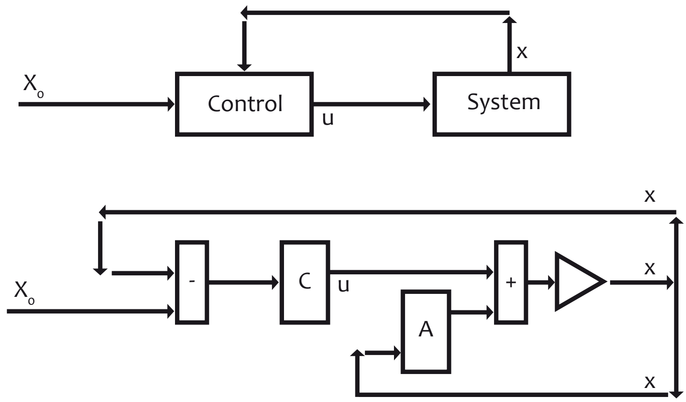

Figure 2.12: Schematic of a control system described above

The above mentioned feedback control system describes the dynamic control aspects of a vast range of systems, from engineering (control of a power plant, speed control), economics and management (all types of control) and cybernetic systems in social, natural and life sciences. From a mathematical system, very general results can be obtained – e.g. on the stability of the system – that will be valid for all kinds of models and systems for which the mathematical system is a model. Note that dynamic systems can also be modelled via dynamic flow models.

5. THE MODELLING PROCESS

For a scientist, models have several important types of usage:

- Models developed by other scientists can be used to do research on the objects that have been described. This is the only case where no modelling process is involved.
- Generic models are used to describe own findings (especially by creating a unique model from empirical findings). This only involves developing a modelled situation through determining model parameters, facts and figures.
- Generic models developed by other scientists can be used to do general research or to adapt these models to develop and use dedicated model instances. This involves some modelling activities on the part of the researcher.
- New generic models or model types are developed as a generalisation of empirical or model-based findings, either as a consequence of combining several models and findings, or as a specialisation of more generic models. This involves the whole modelling process.

According to this, we have several concepts of the process of modelling in science. In general, we can use a linear model of modelling phases, but we have to superimpose a cyclic model for the ongoing process of testing (verification, validation), adaptation and continuous improvement.

5.1 Phases

The modelling process can be executed in several ways. For a linear phase model the following can be used:

- *Pre-modelling, information gathering, problem analysis, system analysis, systems definition*: This phase starts with a real world problem and the modeller gains insight into and information about the problem. The structure and components of the system are identified. By means of abstraction and simplification, an informal model of the relevant real world aspects is created.
- *Model selection*: Starting from the knowledge about a real world system and the problem to be solved (research question), the relevant aspects are determined and an adequate model class is selected. From this, the model is coined by adaptation or created by specialisation. This very generic model is then a more or less formal model, eventually described by mathematical formulae.
- *Modelling, working out structure, notions and parameters*: The structure and the variables of the model are now determined. The parameters of the model are determined by counting or by measurements, or determined as estimates (see the remarks on the measuring process).
- *Analysis, adaptation, refinement and improvement*: The model is now adapted to the real world system by comparing outcomes from the model with real world experiences. Often this leads to an adaptation of the structure and the parameters of the model.
- *Testing, verification and validation*: The final model is now tested against reality to ensure usability. Although a model can only be proven wrong (disproved) by counter examples, the concept is to use a match between a model's outcome and real world observation as a proof for the verification (syntax) and validation (semantics) to ensure usability (pragmatics) of a model.

5.2 The range of models

Especially in complex systems, there is not a single model that can cover all relevant aspects of reality and simultaneously be a basis for problem solving. The concept of essential and physical models leads to different classes of models: while an essential model is rather abstract and can be handled formally, the physical model is much closer to a real world system and contains all relevant facts.

The optimal trade-off (level of formality and abstraction) depends not only on the real world system but also on the intended model usage and on the tools available for analysis or problem solving.

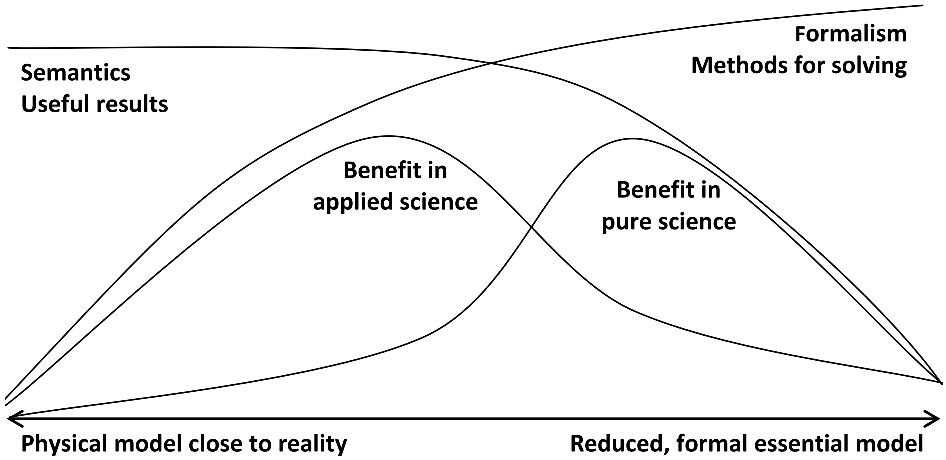

Figure 2.13: Deriving the optimal benefit from models

5.3 The modelling cycle

In addition to the linear model, there is a cyclic process of using, testing and changing the model. Adaptations apply to the parameters or structure, model semantics and syntax and even on the level of generating a new model type. Adaptation may also require integration of aspects of non-linearity, dynamics, stochastics or interfaces (human behaviour) into a model – making it increasingly complex – or to approximate models in order to allow problem solving.

5.4 Modelling aids

In the following section, some practical hints for deriving mathematical models for a problem or system are given.

- *Structure*: A sketch denoting the structure of the research question, and secondly, the objects considered are a good starting point for any problem-solving process.
- *Variables*: When starting modelling, it is important to determine the essential variables with an effect on the outcome of the model. For this, it is helpful to sketch some informal networks – "what is connected to what" – and to ask which variables are pre-defined and which vary within the problem considered. The criteria and decision variables of the system, or simply the question "what do we want to know?" can be used as a starting point in this process.
- *Invariants*: A good approach towards determining relations and structures is to consider what remains constant. These invariants help to identify the important model aspects and variables and also the governing laws. It might assist to consider what differentiates this problem from another similar one, or alternatively, what remains the same.

- *Hierarchical modelling and structuring*: If the system becomes too complex, it can often be divided into smaller sub-systems. This policy of "divide and rule" requires thorough consideration since the relation between the different components or hierarchical levels of the model must also be modelled adequately.
- *Simplicity*: Another important criterion for models is simplicity. Occam's razor: "entitia non sunt multiplicanda praeter necessitatem" means that a simpler model should be preferred. This implies that within the modelling process, the modeller should never cease searching for simpler alternative models.

6. SUMMARY

Modelling is an important research methodology that increasingly finds application in all academic disciplines. Hence, it is a tool that is imperative for all serious researchers with the intention of improving their understanding of any phenomena they are studying.

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CHAPTER 3

Using Mathematical Modelling in Human and Economic Sciences

PG le Roux

1. INTRODUCTION

The usage of mathematical modelling is no longer limited to traditional mathematical related research areas like finance and computing, but it has become a common trend to use this kind of technology in the broader spectrum of the social sciences as well. Mathematicians have had the tools and the ability to perform predictive modelling since the nineteenth century.

An important reason for the creation of mathematical models is vested in the ability to build theoretical models on how an organism, a piece of technology, a group of people, or any other "system", may behave under predetermined, specified circumstances [1].

The recent adoption of mathematical modelling in other diverse areas is the result of society's increasing familiarity with computers. Computer programming in nearly all spheres of life, from chess games and stock price analysis to the most sophisticated medical analysis, contributes to the claim that the world's been hit by a storm of mathematical modelling [2]. From the so-called new world order in the application of models (in the broader sense of the word), modelling forms an integral part and the basis of applied and operations research in the total spectrum of disciplines.

Mathematical modelling in human sciences can include a wide variety of research areas in modern society. The following examples are worth mentioning:

- *Population growth*: Tendencies and influences of population growth on natural resources, the environment, economical and political stability.
- *Economics*: Supply and demand of goods and services, distribution of wealth, pricing, consumer behaviour and fluctuation of the total international financial environment.
- *Politics and social challenges*: The management of conflict, disasters, unstable governments and health and environmental crises.

2. THE IMPACT OF TECHNOLOGY ON RESEARCH IN HUMANITIES

Mathematical modelling, as a tool or mechanism in the operations research process, is designed to explore and understand how social research can contribute to the conceptualisation and implementation of technology in satisfying human needs for the possible prediction situations that may develop, and to assist people/researchers in reaching their goals.

Management and business environments are becoming increasingly more complex and therefore it has become imperative to use all available methods and techniques in the decision-making process. Technological thinking can be regarded as an absolute necessity in the challenging world dominated by the creation of new knowledge – with a focus on the accelerating development of innovative designs in the research process.

3. WHAT IS A MODEL AND THE PROCESS OF MODELLING?

Harper defines a model as follows: "A model is essentially a device that reflects the workings of the real world" [3] while modelling refers to the process of generating a model as a conceptual representation of some phenomenon. Typically a model will refer only to some aspects of the phenomenon in question and two models of the same phenomenon essentially may be different, that is in which the difference is more than just a simple renaming. This may be due to differing requirements of the model's end users or to conceptual or aesthetic differences by the modellers and decisions made during the modelling process [4]. In short, modelling is the art and science of constructing models. Models can be classified in two major categories:

- *Physical*, as in a model airplane or architect's model of a building, or
- *Symbolic*, as in a natural language, a computer programme, or a set of mathematical equations.

According to Harper, the type of model most frequently used in operations research is, however, a *mathematical model* [3]. That is a model that reflects the working of the real world by means of mathematical symbols and formulae. Mathematical modelling refers to the use of consequential mathematical formulae to create a numerical model of the possible events in a system. Introduction of a series of values for individual variables makes it possible to produce a series of results that mirror the outcome of practical experiments [5].

The figure below illustrates the process of observing the system, collecting the consequent data, feeding that data into the mathematical model and possibly using analysis of the model to adjust the data collection [6] and the interpretation thereof.

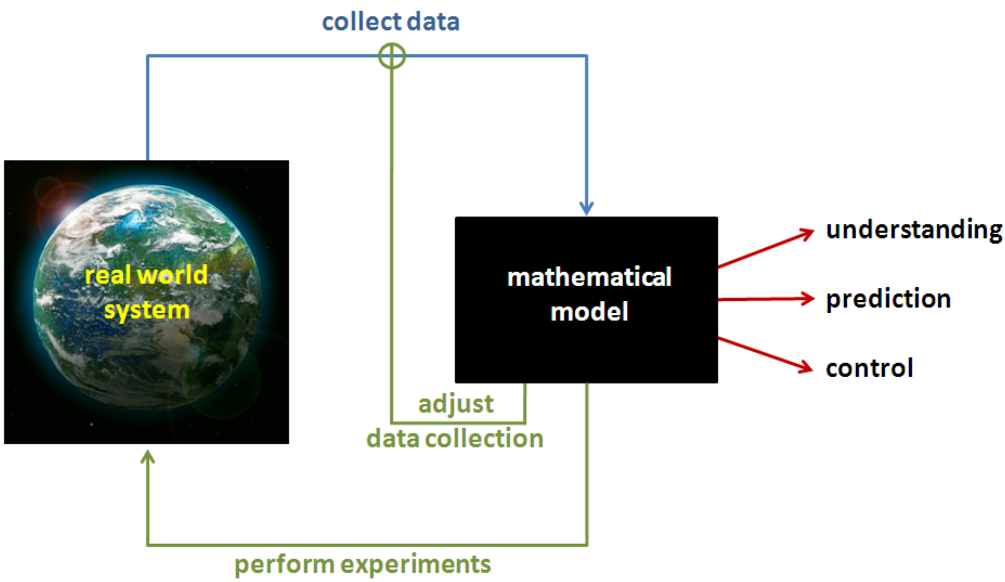

Figure 3.1: Collecting data from an observed system, feeding it into a mathematical model, adjusting the data and the interpretation thereof

4. PROCESS APPROACH AND MATHEMATICAL MODELLING IN BUSINESS AND HUMAN SCIENCES

Operations research involves "research on operations" – so to speak operations research is applied to problems that concern how to conduct and coordinate the operations/activities within a given structure. The primary purpose of operations research is obviously to see if it is possible to identify the best way of operating in a particular context. In a nutshell: *operations research* (terminology used in USA, Canada, South Africa and Australia while Operational Research is used in Europe) is the discipline of applying advanced analytical methods to help make better decisions. In some cases it is defined as the science of decision making.

This interdisciplinary branch of applied mathematics and formal science uses methods such as mathematical modelling, statistics and algorithms to arrive at optimal or near optimal solutions to complex problems. The process of scientific modelling (in general) normally consists of generation of an abstract, the conceptual phase, and graphical and mathematical model building. The boundaries between the different steps or phases are often blurred, which can impact negatively on the scientific outcomes of the project.

The following process analysis is an attempt to standardise the procedure for the application of a typical mathematical model in an operations research exercise [7].

4.1 Define the problem of interest and gather relevant data

Problems that are vague and imprecise should be avoided. Clear identification of the problem, and the objectives of the study and relevant and accurate data about it, is regarded as a prerequisite for success.

The use of appropriate computer-based management information systems (MIS) will assist to improve the precision of the data.

4.2 Formulate a mathematical model to represent the problem

The development of a symbolic representation of the real situation is the first creative step in selecting a "correct" model or the best appropriate model representing the system.

The application of mathematical models and the use of high-powered mathematical techniques are much more reliable and concise than verbal descriptions. Ideally, there should be a high correlation between the prediction by the selected model and what would actually happen in the real world.

The dynamic nature of the process should allow model enrichment as long as the model remains tractable.

4.3 Develop a computer-based procedure for deriving solutions to the problem

Well-designed mathematical models aligned with mathematical procedures are important in finding proper solutions. Software packages are available for standardisation of the procedures and calculations which are normally too expensive to be done by hand.

A well-structured computer-based procedure also allows the researcher to set certain goals in order to establish minimum satisfactory levels of performance. In the search for the optimal solution ("science of the ultimate") the computer-based process can be regarded as the most cost-effective method.

4.4 Test the model and refine it as needed

Check and test the model for sufficient and accurate representation of the real problem. The two most relevant questions at hand are: does the model provide reasonable solutions, and: are the solutions provided applicable?

Model validation (the check for obvious errors, oversights and if mathematical expressions are dimensionally consistent) could be regarded as the most important link in the quality assurance process.

4.5 Apply the model to analyse the problem with recommendations

Verified data as output from the Management Information Sysytem (MIS) provide various versions of the model and permutations of the so-called decision support system to support the decision-making process.

4.6 Implementation of the model

The final stage is the implementation of the model with recommendations and modifications as approved, and the monitoring of the initial experience with the newly created system [8].

The theoretical process explained above is often fast-tracked by a more practical approach in a real problem-solving situation. The flow chart shown in Figure 3.2 illustrates the process.

5. ESSENTIAL CHARACTERISTICS OF GOOD MATHEMATICAL MODELS IN THE MANAGEMENT SCIENCES

The goal of the scientific method is to simplify and explain the complexity and confusion of an identified problem. The researcher then uses the model of science to predict, analyse and solve the problem.

For mathematical models to be useful in the application of operations research within the human and business sciences, the following characteristics are essential.

5.1 Simple

Simple models are more easily understood by the problem owner or decision-makers, who are often mathematically untrained. It is often not possible to avoid complicated mathematical models, but easier to follow the logic of a spreadsheet. The ultimate goal of the researcher is to create simple models that have a great deal of explanatory power.

In most cases, simple and powerful models are not yet available to the researchers in the social sciences. A trade-off occurs between the power (impact) of the model and the number of simplifying assumptions made about the research problem. A researcher in the social sciences must decide at what point the gain in the explanatory power of the model no longer warrants the additional complexity of the model.

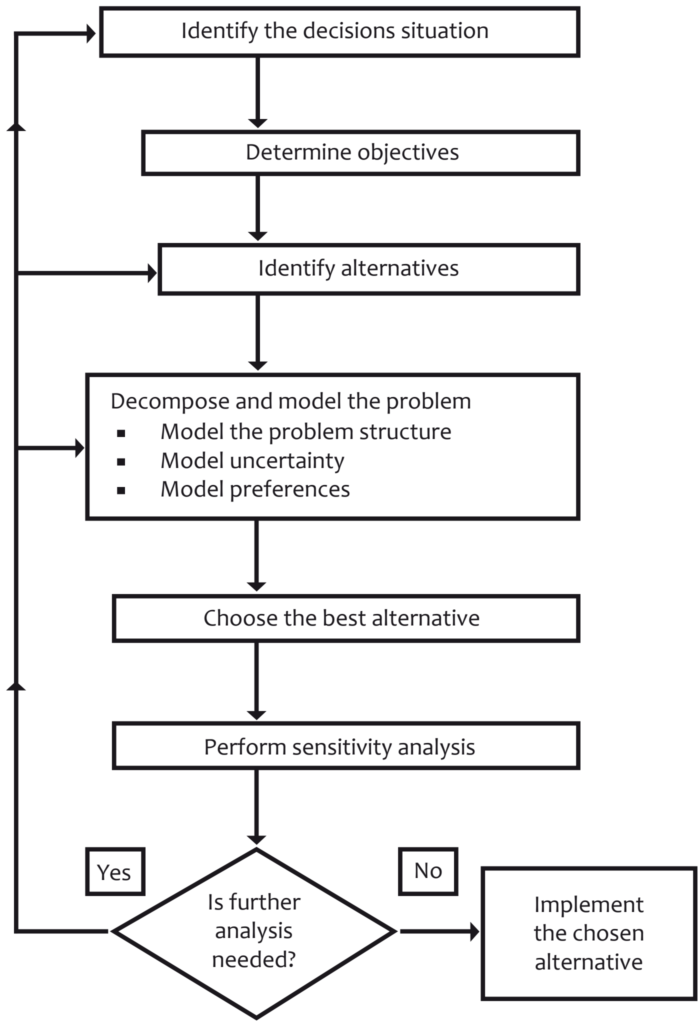

Figure 3.2: Development and implementation of a mathematical model to assist with decision-making – as shown in [9]

5.2 Complete

A model is necessarily incomplete because it is a representation of reality. The model should reflect all (as far as possible) significant aspects of the problem statement. The key issue here is to know, before the model is designed, whether all aspects are likely to affect the optimal solution in a significant way.

5.3 Easy to manipulate

It should be possible to obtain answers from the model with a reasonable amount of computational inputs. The best solutions flowing from the model should be achievable in an acceptable time frame. Changing or manipulating symbolic models is generally much easier than changing physical models.

5.4 Adaptive

If change in the structure of the problem situation invalidates the model, it should be possible to adapt to the new situation with relatively minor model modifications.

5.5 Easy to communicate with

Interactive user-friendly computer programmes and software, with good representation of the results of the modelling process, are preferable for use by mathematical modellers. The model owner is therefore looking for confidence and credibility in the model and the modelling process. The first prize would be to talk about desirable properties of the modelling process.

5.6 Appropriate for the situation (problem) studied

In essence, the model must deliver the relevant outputs at the lowest possible cost and in the appropriate time frame required for effective decision-making.

5.7 Produce information that is relevant and appropriate for objective decision-making

This means that the output of the model has to facilitate a direct influence on the decision-making process without any further extensive translation or manipulation. The information should lead to insights and conclusions that the decision maker could not easily obtain by other means [10, 11].

6. SCIENTIFIC AND MATHEMATICAL MODELLING IN THE SOCIAL SCIENCES

The field of research in the social sciences concerns the broad question of "the human" as the subject of inquiry. Anthropologists, sociologists, economists etc. define its contours as a specialty in the exploration of a variety of topics in the characterisation of human nature. Mathematics offers the technical tools for students of the above-mentioned disciplines to make models of phenomena of interest. Mathematical models in anthropology, physics and economics are familiar – if not in detail then at least for their important role in establishing some predictive power and thereby credibility and status for the discipline.

Models in social sciences are sometimes regarded as stepping stones or mediators between the world (practice) and theory. Predictive power is not necessarily explanatory power. The application of model/mathematical models in human science research is often accompanied by the telling of an informal "story" concerning the context, mechanisms and consequences of the problem under investigation. It is about discover, invent and learn in a language that offers a precise, clear representation of a problem situation [12].

7. MODELLING IN THE ECONOMICS – A CONSTRUCT FOR DECISION-MAKING

Economics is the social science that studies the production, distribution and consumption of goods and services. Economic methodology is the study of methods, usually scientific methods, in relation to economics, including principles underlying economic reasoning [13].

In economics, a model is a theoretical construct that represents economic processes by a set of variables and a set of logical and/or quantitative relationships between them. An economic model is therefore a relatively simple representation of a set of complex real world relationships. It is “a logical representation of the essence of a situation” which eliminates insignificant or inconsequential detail, leaving the core of the problem exposed for analysis.

Generally speaking, economic models have two functions:

- Firstly, as a simplification of, and abstraction from, observed data. Overly complex models are often of little practical use. The more complex the model, the more difficult it is to communicate the results. The skill in model formulation is to be able to achieve the right balance between practicality and complexity.
- Secondly, as a means of selection of data based on a paradigm of econometric study. Selection is important because the nature of an economic model will often determine what facts will be looked at. Effective models capture the essence of the economic issue without drilling down in minor detail.

In the economic modelling process (normally), the relationship amongst economic variables, implied by theoretical arguments, is expressed by mathematical symbols and equations. This form of representation is very popular as a technique of modelling in industry and business, since a mathematical model describes a problem concisely and forms a bridge to use high-powered mathematical techniques and computers to analyse a problem.

The application of mathematical modelling in an economic environment is normally used for:

- *Business insight*: Providing quantitative and business insight into complex problems.
- *Business performance*: Improving business performance by embedding model-driven intelligence into an organisation’s information systems to improve decision-making.
- *Cost reduction*: Finding new opportunities to decrease cost or investment.

- *Decision-making*: Assessing the likely outcomes of decision alternatives and uncovering better alternatives.
- *Forecasting*: Providing a better basis for more accurate forecasting and planning.
- *Improved scheduling*: Efficiently scheduling staff, equipment, events, and more.
- *Planning*: Applying quantitative techniques to support operations, tactical planning, and strategic planning.
- *Pricing*: Dynamically pricing products and services.
- *Productivity*: Helping organisations find ways to make processes and people more productive.
- *Profits*: Increasing revenue or return on investment; increasing market share.
- *Quality*: Improving quality as well as quantifying and balancing qualitative considerations.
- *Recovery*: Gaining greater control and achieving turn-around.
- *Resources*: Gaining greater utilisation from limited equipment, facilities, money, and personnel.
- *Risk*: Measuring risk quantitatively and uncovering factors critical to managing and reducing risk.
- *Throughput*: Increasing speed or throughput and decreasing delays [14-16].

8. MATHEMATICAL MODELLING – A PRACTICAL APPLICATION TO A REAL PROBLEM IN THE SOCIAL AND ECONOMIC ENVIRONMENT

The use of mathematical modelling is no longer limited to traditional mathematical-related research areas like physics and engineering. It has also spread to areas like finance and computing and it has finally become common practice to use this kind of technology in the broader spectrum of the social sciences as well.

The following describes a practical application of a mathematical model that was used to resolve a typical economic problem, namely the optimal utilization of passenger seats on an aircraft.[1] The study was done by Dr. Christine Currie as part of the Millennium Mathematics Project of the University of Cambridge - see [17].

8.1 Differentiated Pricing

Any business has the challenge of trying to optimize its income. In the case of an airline, it strives to sell all the seats available on any flight at the highest possible price per seat. However, since the importance of being on a particular flight, as well as the individual financial situation of potential customers, differs from one individual to the next, there is not a uniform amount that all potential travellers are willing to pay for tickets on a particular flight. Hence, over a period of time

1 This section illustrates a typical application of modeling as referred to in Chapter 2.

airlines developed a system of differentiated pricing where the maximum number of tickets is sold at the highest possible price, whilst the remaining tickets are sold at a reduced price. These discounted tickets are sold subject to certain, specified restrictions. In this manner an attempt is made to fill the maximum number of seats at the higher price and all remaining seats at the discounted price. Obviously if too many seats are sold at the lower price, there would not be enough seats available for all those who would have been prepared to pay more – hence, the airline's income would not be maximised. A similar situation would arise if too few less-expensive seats are sold since this would result in a situation where the available number of available more-expensive seats would exceed the need for such.

8.2 Understanding the customer's needs

In order to successfully optimise its income from ticket sales, airlines need to be well-informed about the travelling needs and financial means of its potential customers. Theoretically every potential traveller has a reserve price for a particular flight. This is the maximum amount the customer is prepared to pay for a ticket. However, airlines are not informed about the reserve price of any individual, it has to determine from historical data on similar flights what customers might be willing to pay to make a trip. In this manner the airlines may develop a better understanding of the preferences and needs of passengers.

The less-informed an airline is about the reserve price of travellers, the greater the likelihood of either not all tickets being sold at the maximum possible price, or some tickets are not sold at all. Both these scenarios would result in the situation where the airline could have earned more. The only way in which this can be avoided is for the airline to try and determine a general reserve price – since each individual has a particular reserve price, the process invariably leads to a generalised approximation the actual reserve price - as accurately as possible.

Airplane ticket sales are very cyclic with certain flights being very popular and others relatively unpopular. The nature of this tendency depends on several different phenomena such as the time of day – with business men who travel to a certain destination in the morning and would prefer to return home the same evening. Similarly, business trips often last for approximately a week, with people departing late Sunday afternoon or Monday morning and returning Friday afternoon. Obviously there is also a huge increase in travellers over long weekends or during the holiday season. Hence forecasts of the number of potential travellers and their relative reserve prices need to be determined from previous flights under similar circumstances long before any particular flight and as accurately as possible.

8.3 The Problem of Maximising Revenue

Any aircraft has a limited seating capacity, the primary constrain that has to be taken into account in the optimisation of the of airline's income from a specific flight. This has got to be aligned with the potential customer's reserve price for the flight. The following is a simplified example to study the kind of problem that airlines face on a daily basis.

In practice there are typically more than two prices that customers would be expected to pay, depending on their individual situations. Yet, for the sake of simplicity the scenario will be created for a hypothetical flight where only two fare rates are available. It is further assumed that the airline has a good estimate of what the expected demand for the two types of tickets will be and that the demand is deterministic. It would now be possible to solve the problem exactly by writing the optimal revenue problem in the form of a number of linear equations.

The total revenue would equal the sum of the income from the higher-paying customers and that of the lower-paying customers. This can be written as:

$$a = p_l s_l + p_h s_h$$

where p_l and p_h indicate the price of the lower- and higher-priced tickets respectively. Similarly s_l and s_h represent the number of seats sold at lower and higher prices respectively.

The sale of seats should comply with the following set of constraints [17]:

- "We cannot sell more tickets than we have seats on the plane (actually airlines do sometimes ignore this constraint – a technique called overbooking …), therefore, $s_l + s_h \leq C$, where C is the number of seats on the aircraft.
- The number of low-cost seats sold must be less than or equal to the demand for low-cost seats: $s_l \leq d_l$.
- The number of high-cost seats sold must be less than or equal to the demand for high-cost seats: $s_h \leq d_h$."

In short, as many as possible seats should be sold at the higher price, whilst all the remaining seats must be sold at the lower price.

The respective number of seats in the different categories, s_l and s_h, are called decision variables and can be controlled by the airline. By using linear programming the optimal values for these variables can be determined whilst ensuring that all of the above constraints are obeyed. For the present example, a diagram as shown in figure 3.3 can be drawn. This shows the implementation of all constraints.

From figure 3.3 it is obvious that to maximise the revenue, s_h should be determined such that all the available high-fare paying customers are accommodated in high-cost seats. All the remaining seats should be filled up with passengers paying low-cost fares.

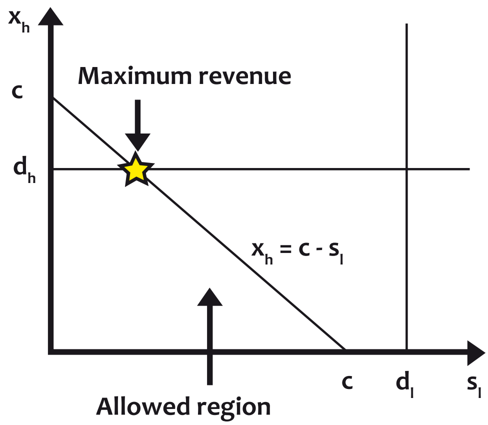

Figure 3.3: Plotting of different variables to assist in decision making [17].

8.4 Adding More Complexity

Actually the airline not only has to decide on the ratio between lower- and higher-priced tickets, but also on the actual fare to charge for each category. However, the actual value of none of these four variables - two sets of two variables each - is not known precisely. Hence expected values have to be determined using actual situations that happened in the past under similar circumstances and probability distributions. This is not a simplistic matter and ideal solutions are often not reached.

In practice the above describes a very much simplified approach to the problem. Typically airlines would rather consider their preferred price for each individual seat as belonging to one of, say, ten groups, rather than simply creating two categories of seats with different prices. Hence a wide variety of different prices is normally applicable on any flight for both economy and more expensive classes of travellers. In an effort to motivate customers to purchase the most expensive category of seat possible, each of these categories will have slightly different conditions applicable to it – the cheaper to more constrained. In turn, the airline has to decide on the actual price and number of tickets reserved for each of the categories of tickets. The cyclic principles referred to above are used to regulate the extent to which the different prices are determined.

As indicated most airlines generally make use of a system of overbooking whereby more tickets are sold than what are actually available on the particular aircraft. The reason for this is that it is very common for some potential travellers not to turn up for a flight. This may be due to factors such as passengers falling sick, meetings that run over time or problems with traffic on the way to the airport. An obvious consequence of this system is that occasionally more travellers may turn up for a flight than the number of available seats, causing a lot of inconvenience and possible payment of some compensation by the airline to these passengers.

Even though it creates some tension and unhappy passengers, the system of overbooking is fully entrenched in the booking system of modern airlines in an effort to maximise the revenue of airlines.

One of the newest developments in modern passenger aviation is the establishment of low-cost airlines. These entities provide a very inexpensive service at the cost of additional luxuries such as meals and reservation of specific seats. This simplifies the problem of price determination drastically since normally the only factor determining the price of a particular ticket now is the period between the purchase of the ticket and the flight. However, especially in some countries, the tendency is for airports to limit the timeslots for take-off and landing for these airlines to less acceptable times.

8.5 Hub-and-Spoke System

Increasingly the number of flights landing at any airport, or departing from such, is limited by the limited availability of runways rather than the number of potential passengers. The tremendous growth in air travel was accompanied by increasingly complex flight preferences of passengers where an increasing number of smaller venues must be serviced regularly. This created a situation where increasingly use is made of the so-called hub-and-spoke system with an extremely complex system of interconnecting routes. Hence it is now common for travellers to fly on a connecting flight from a smaller airport to a major airport, and from there onwards to the passenger's actual destination, or perhaps even after only another connecting flight. This type of service is often shared between airlines working collaboratively. Hence it is no longer only different airlines servicing the same routes, but also an increasing number of formal alliances between groups of airlines that are able to provide the fastest, most convenient service to customers.

Understandably the hub-and-spoke system add more complications to the revenue optimisation problem – a critically important problem for airlines that are often financially challenged due to many operational parameters which are beyond their control, such as rising oil prices.

8.6 Not Just Airlines

The practice of a mathematical approach to the determination of the pricing of products is not confined to airlines only. All of the principles discussed above are as applicable to any highly competitive industry operating on fast turn-around times such as hotel rooms, car rentals, airport parking, etc. Even the sale of perishables such as beef and vegetables can be optimised using the specialised income management processes. In fact, the sale of any set of identical products with an expiry date and limited capacity could be optimised using income management [17]. However, it is appreciated that due to the relative complexity of such a system it would be most unusual to find it implemented in a relative small commercial enterprise or to manage the sale of less-critical products.

9. SUMMARY

In recent years, there has been an increasing demand by researchers to apply the technique of mathematical modelling in business and management related research projects. Recent developments in computer technology and related software have provided the necessary tools to assist researchers from the social sciences with their decision making processes. The expensive traditional method of trial and error experimentation has now been replaced with a more flexible and cost effective approach through the use of mathematical modelling and computer simulation.

The major weakness of mathematical modelling is the fact that this approach does not have intuition or feeling, but this is also the strength of this research method. Using technology (to assess all the options fast) instead of human decision making might be the best way to take a well informed decision. The total elimination of the human factor specifically in the human sciences is beyond the point of debate. Mathematical modelling is a great support for decision making and planning, as long as the emotional intelligence component of the researcher has been added.

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CHAPTER 4

Models in the mechatronic design process

Peter Hehenberger

1. INTRODUCTION

Especially in today's economic environment with its global competition and high dynamics, a superior design concept for a product is crucial as it pre-determines the main element of success of the product. For any new product, the question is less how to realise it, than to find a promising superior product concept. In the traditional linear model of design, the process flows from synthesis through analysis to evaluation. Design methodology at the conceptual level includes the creation of innovative concepts, comprising a description in low detail but with sufficient relevance for evaluation of their essential properties in comparison to other concepts. The main properties (parameters, costs, etc.) of the product are fixed during the conceptual design phase in the product development process.

When a totally new system (an overall system, sub-system or component) is designed, the conceptual design process leading to the design concept for the system is usually a mentally intensive and challenging activity. As this step fixes the main element of success of the new product, it should be done by expert engineers. Due to mechatronics, the toolbox of solution principles is widely extended; hence, the variety of different solution concepts is drastically increased. This is the reason why conceptual design of mechatronic systems will be investigated in more detail.

Amongst the spread of information available to the designer, standards, directives and supplier data generally provide specifications and specific aspects of products and their requirements. At the same time, the engineer has to follow several design rules representing general information. Both aspects require a more detailed knowledge of the structure of the product to be developed, of its functions and production in order to make reliable predictions regarding the properties and cost of the product. Although the characteristics of the product are influenced to the greatest extent during its design, the information for design, as a general rule, is mainly derived from experience that can only be gained from the phases of the product life cycle following design.

2. CHARACTERISTICS OF MECHATRONIC SYSTEMS

2.1 Definition of mechatronics

Mechatronics can be considered to be an integrative discipline utilising the technologies of mechanical engineering, electrical/electronic engineering and information technology in order to provide enhanced products, processes and systems. The role of mechatronic subsystems will increase dramatically in future product development processes. Two of the main driving forces for this development are the improved functionality of mechatronic products with increased complexity and the resulting demand for modularisation [2, 3 and 7].

The high integration in design allows the realisation of a great variety of required functions in a single mechatronic system - which often results in an ideal tailor-made design with respect to the given requirements - but it has disadvantages when this system should be reused for other design tasks. There is a demand for modularity in product design, which means that a mechatronic module should preferably be exploitable repeatedly for many different tasks.

In a mechatronic design process especially the phase of conceptual design is crucial. Here the functional interactions between domain-specific subsystems are determined and have to be investigated carefully. This implies that during the phases of conceptual and preliminary design the designer should be able to quickly and accurately evaluate the system's potential performance due to design changes in the mechanical part as well as in the other parts (electronics, software etc.). With a mechatronic approach, mechanics and control aspects are studied simultaneously.

2.2 Mechatronic design

Mechatronics design is the competence of integration between mechanics, electronics and software.

As new functionality in products is realised to a large extent through integration of mechanics, electronics, and software the need for knowledge integration between these disciplines becomes central. Design of embedded systems such as intelligent sensors, communication and power systems needs to be integrated into mechanical design, and also be developed to be maintained and recycled. Software and hardware platforms change due to new technology and new technical interfaces emerge which lead to new challenges for the research and development function. The interactions between product developers from the different disciplines are hindered by insufficient understanding between the disciplines and by missing common platforms for modelling of complex systems. As many sub-systems are delivered by suppliers, there is a need for both a horizontal integration within organisations and a need for a vertical integration between the sub-system suppliers and the suppliers of full systems [1, 4].

The increasing use of computers and electronics, as well as their continuous enhancement, has led to an increase in the complexity of the product design process itself. Due to the different disciplines involved, the mechatronic design process may become very complex. Hence, a new approach to the design and engineering of products can be considered as a key point to optimise the design process.

Specific design tools are required to support the engineer in solving mechatronic design tasks, with their specific properties being in particular:

- the functional interaction between domain-specific (discipline-specific) components, which is the key to any mechatronic solution;
- the selection or alteration of a solution in one domain which may affect the solutions in other domains; and
- the prediction and evaluation of the system performance of a particular solution, which implies the investigation of the system components from other domains (disciplines) as well as their interactions. This makes it difficult to guarantee the specific performance of a new mechatronic system in advance.

One of the key issues in the development of modern mechatronic systems is the strict integration of mechanical, control, electrical and electronic aspects from the beginning of the earliest design phases on, as can be seen in Figure 4.1.

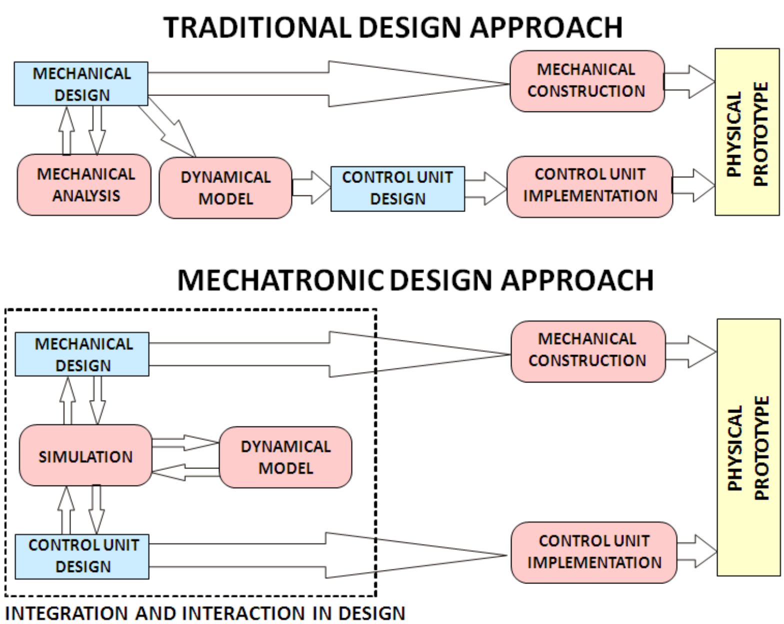

Figure 4.1: Comparison between the traditional and mechatronic design approach

The key to an integrated mechatronic design methodology is modelling and simulation. In this context design models and their inter-changeability between different design tools are very important during the design process. From the mechatronic design process viewpoint, models are containers of the knowledge of the product during its total life cycle. Simulations produce information on the design problem. This may improve product knowledge and potentially also the quality of many analyses and decisions. The presented approach relies on modular model architecture and enables innovative design, flexibility, speed and assistance in non-routine design questions.

A particular design methodology has been introduced by the Association of German Engineers - the VDI - for mechatronic systems and suggests the carrying out of the development process of mechatronic systems according to the so-called V-model (Figure 4.2) [10].

After analysing all requirements of the total system, the sub-functions and sub-systems are defined (left branch of the V-model). They are to be developed simultaneously by several cooperating development teams. After verifying the sub-functions and testing the sub-systems, they are integrated step by step (right branch of the V-model).

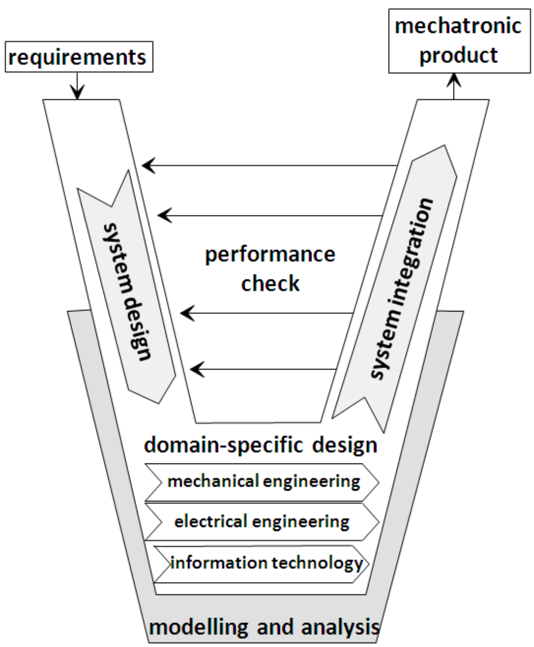

Figure 4.2: The V-model for the design of mechatronic systems

2.3 Organisation of mechatronic design processes

Many researchers have carefully analysed the different steps during the design process [8, 9 and 11]. The development / design process is usually structured into four sub-processes [8], namely the phases of Problem Definition, Conceptual Design, Preliminary Design and Detailed Design.

The explosion of information technologies in the recent past has also revolutionised the design process. The information technologies provide new tools for communication in the development process. Databases and CAD systems provide reproducible, "error-free" archives and design baselines of the product instantly accessible for all authorised design engineers. Information technologies also provide a useful window into the team and design process for analysis and tuning of the design activities. These new technologies, of course, require specific training.

Another important aspect is the consideration of technical and social interaction in design teams. For mechatronic projects, experience in the interdisciplinary nature of the design process plays an important role. Conceptual Design is one of the most important phases during product development, as the main parameters, properties and costs of the solution - and consequently also the main elements of success of the new product - are fixed here. When a completely new system (overall system, sub-system or component) is designed, the conceptual design process leading to the design concept for the system is usually a mentally intensive and challenging task. As this step fixes the main portion of success of the new product, it should be done by expert engineers.

The determination of the product's overall function and of its most important sub-functions (main functions) and their interaction, leads to a functional structure. During this design phase, principal solutions with a structure of realisable modules should be established.

In this stage cooperation between the different design engineers is of vital importance for the success of the design process. Typically, the mechatronic design team consists of several engineers, possibly organised in domain-specific teams. Each engineer is an expert for some of the subsystems or disciplines that make up the system design, with responsibilities for all the design aspects related to the subsystems under consideration.

2.4 Design models

During all phases of the design process there is a need to create models which may be seen as simplified representations of the real world. During different phases, these design models serve different purposes. During the conceptual design phase, physical principles, functions, structures, etc. have to be evaluated by building models. In most cases, analytical and virtual models are less expensive and less time-consuming than physical prototypes. Virtual models can be implemented - and even integrated - and used to simulate and evaluate (significant representations of) reality with the help of computers.

A model is a conceptual description of ideas, facts and processes that together represent (describe) the operational model of a designed product [12, 13]. A design object may be an assembly, subassembly or a single component, represented by the product structure model. In general, a mechatronic design model is devoted to the task of mapping reality onto a significant representation of reality, in order to make valid predictions about reality. It should include the relevant effects of interest ("views of the object") such as geometry, dynamics, stability, materials, electro-dynamics, controllability, cycle time, maintenance etc.

Design models may be used for the evaluation of different solutions during the design process. At least for this step, quantitative models are indispensable, parameters being the decisive elements to provide an adequate quantification of design models.

Mechatronic models are very important tools for complex activities such as engineering design. For high performance of the engineering of design tasks, numerical modelling and simulation, i.e. experimenting with computer-based models, are increasingly important problem-solving techniques. The preliminary design phase is often characterised by a cascading series of what-if questions. Some of these questions reflecting requirements may be of controversial character by their nature, and are related to complex dependencies between shape, topological structure, strength, performance, physical behaviour, etc. The complex nature of engineering design, as well as the time- and cost-constraints on the process, requires highly efficient and flexible procedures to configure system models.

3. MODELLING OF MECHATRONIC SYSTEMS

3.1 Requirements and characteristics

Today´s products of mechanical engineering (machine tools, vehicles, aircraft plants, industrial plants, etc.) consist of multiple systems, aggregates, modules and components. They include power over general systems engineering, electrical, hydraulic and pneumatic drive systems, automation equipment including sensors, actuators and regulatory bodies and are often very complex mechatronic systems. Crucial to the success of such a product is the behaviour of an integrated whole, as customer requirements and desires essentially always focus on the whole system, rather than relate to subsystems or even individual components. To assess the characteristics of any system it is appropriate to use models. For modelling and the description of a mechatronic system, it is necessary to limit the system's complexity by considering suitable subsystems, because this describes the boundary of the considered mechatronic system to its system environment (e.g. conditions).

Their functions are distinguished from other systems, enabling a clear definition of interfaces and areas of responsibility. It must therefore be clarified in what way it interacts with the system environment (e.g. chemical, energy, information). The system limits are reasonable so as to define that the pairings for the system environment are much weaker than the pairings in the interior of the system.

Ideally, the whole system is in the form of a cross-domain model, but the problem is that the integration of models of different disciplines, different modelling approaches and models or model descriptions, still leaves a lot to be desired. Moreover, within the individual disciplines, information and highly detailed data that are only partially required in other disciplines, are needed. The objective now is a system model to create information that depicts the various domains, which are important for other domains. The challenge is that the knowledge of the entire system does not equal the sum of knowledge from the corresponding domains. The domain knowledge must therefore be generalised (abstracted) and integrated.

3.2 Definition of a system

The system environment is everything that will not be involved in the system. The system boundary describes the limit of the system to its system environment, with which it has interfaces (e.g. energy or information as well as inputs). The system boundary is often not identical to the physical limits of a system or its components. Its function is distinguished from other systems and hence the clear definition of interfaces and areas of responsibility is necessary. Conversely, by changing the system, limited visibility of a problem can be expanded.

A subsystem is an element of a system (system element), where a system consists of several elements. System elements are thus one component (a building block) of an overlying system and other systems. The decomposition of a system into the system elements and defining relations between them and with the system environment creates a hierarchical structure of the system.

Inputs to a system can be defined as the external relations of the system. Output parameters are the ratios of the system environment and can be measurements, observations of the system, or the activation of physical actions by the system.

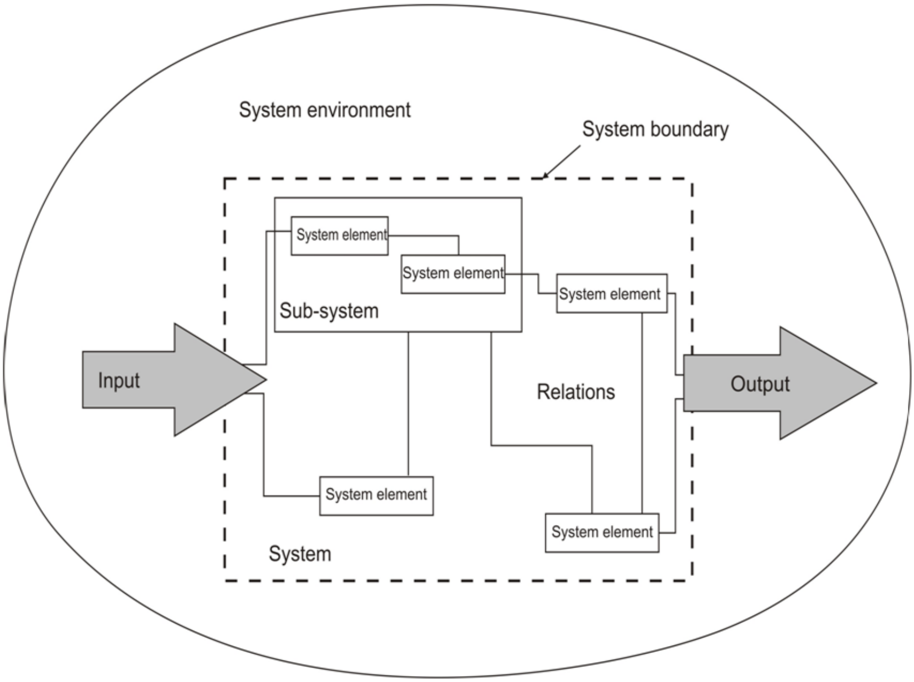

Figure 4.3: Components of a system

A system structure includes the set of system elements as well as a number of relations amongst them and with the system environment. Especially for complex systems, it is useful to define different viewpoints of a system (aspects such as geometry, location, material flow, energy, etc.).

3.3 Modelling of systems

Since the uncertainties in a detailed model of a product under development may be so great that the benefits compared to those of a simpler model are insufficient, very accurate modelling is often not necessary. Models have to be clearly defined and described in a consistent manner and must be manageable so that they are suitable for serving a specific purpose.

There are different ways of modelling a system. However, the principles of model efficiency dictate that the simplest model which will suffice should be preferred. For the building and usage of a simple, efficient and valid model, there are no formal rules, hence previous experience plays a major role. Some building criteria for model structures are as follows:

Design phases

For different phases of the product life cycle, models with different objectives and detail are required. The need for some models is particularly high in certain, very specific stages of the product life cycle (e.g. requirement models, design sketches, models for simulation). In the concept phase, very rough models are typically useful, as they are still based on incomplete information; however, during the design and development phase, the models become increasingly detailed and refined - thereby increasing their information content.

Integration and modularisation

It is appropriate to divide complex machines into installation sections, spaces, design and processing zones, assemblies, subassemblies, structured individual components, etc., where relationships exist between them. In complex systems the modularisation facilitates a systemic overview and more transparency, whilst allowing for parallelisation of the work throughout the product development process. The decomposition of the system into modules and its representation by models also leads to a modular structure of the overall model. For the investigation of systems and system elements, it is always necessary to "virtually" interconnect sub-models so as to portray the operational characteristics of the interfaced sub-systems.

Disciplines(domains)

The investigation of systems requires the treatment of different, very specific views of the system (system aspects) arising from different needs of the different professional disciplines (domains).

3.4 Hierarchy of parameters

It is very useful, if not imperative, to determine some important parameters at an early stage of the design process. A series of design decisions bring a system from the initial design stage, through several intermediate design stages, to the output of the design process, viz. the complete final documentation defining the product comprehensively. The initial design, as well as the design goals, is generally described in vague terms and not definitive. This is one of the reasons why, in many applications, the number of model parameters (MPs) to be fixed is much higher than the number of well defined requirements. Some of the initial, "superfluous" parameters are indeed not essential for the solution (e.g. the height of a shaft's shoulder), but others give rise to optimisation potential of the solution (see Figure 4.4).

The process of defining hierarchical levels must be repeated until elementary solutions (preferably standard components) with their associated, well-known MPs are achieved. This means that we have to switch between the functional and the physical approach during the product development process. The model parameters at any one level can be classified into two categories, where one subset comprises the external parameters representing requirement parameters for the next level. The other parameters are exclusively local at the active level for dimensioning the component at this level (internal design parameters).

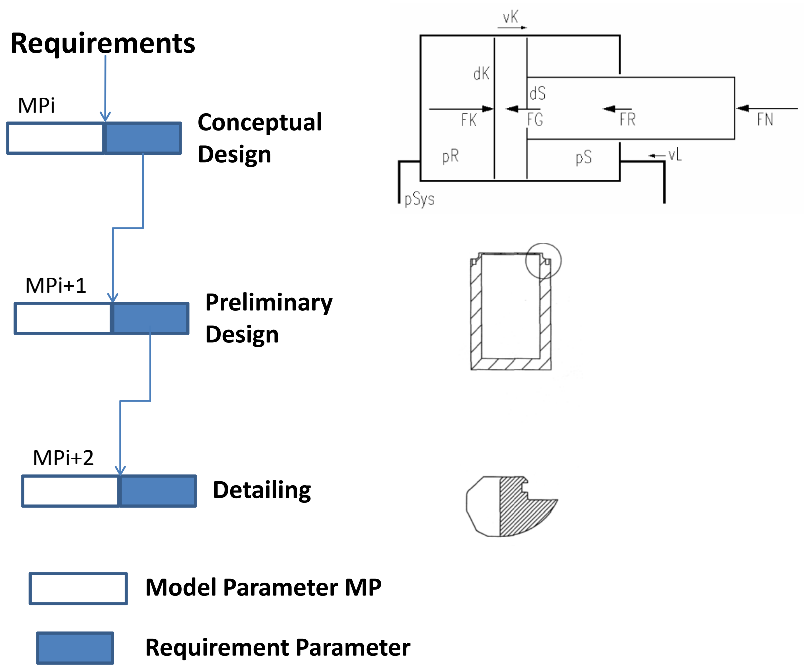

Figure 4.4: Parameter hierarchy

4. APPLICATION OF MECHATRONIC SYSTEM DESIGN

Figure 4.5 illustrates the concept of mechatronic system design by means of an example. The example presents a clamping device. The positioning and configuration of clamping devices, used in various machines or stations of a production line for car bodies, is a recurring question from automotive engineering. Clamping devices are used to fix different sheet metal components quickly to one another in an exact position and with a pre-defined clamping force. After the parts are positioned and clamped, they are joined together (e.g. by welding). Important design requirements for such fixing units are closing speed, compact physical size, and reliability.

When most of the relevant knowledge regarding the new clamping device has been acquired, it is unstructured and needs to be organised and structured, using representations that both computers and humans can understand. Such representations are named "knowledge worksheets". For the mechatronic ontology, we define six concepts, such as "mechatronic device", "environment", "material", "property", "function" and "manufacturing process". In general, each of these concepts is connected with the other relevant concepts through specific relationships.

For instance, a mechatronic device concept (e.g. a gripper) is related to the environment concept (e.g. its connection to a robot arm). The name of the relation is “interaction-with”. The definitions of the relationships that are being used are given as “has-part”, “interaction-with”, “has-material”, “has-function”, and “has-process”. The concepts and their relationships describe the relevant knowledge of a new design concept.

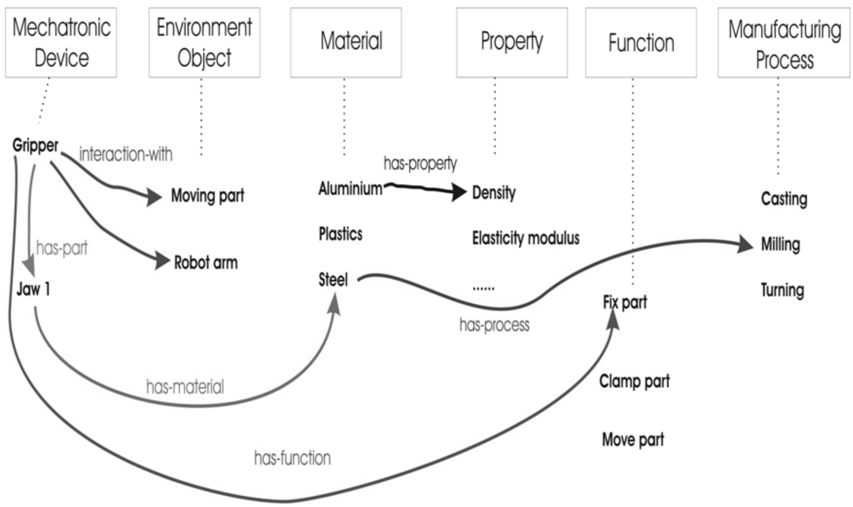

Figure 4.5: Application gripper: system description

Figure 4.6 shows the gripper in more detail. According to the mechatronic pillar model principle, which helps the engineer to analyse and evaluate functional requirements and design parameters of possible solutions [5, 6], we decompose this design problem into three domain-specific components and their hierarchical levels. One pillar characterises the mechanical components, such as material, geometric dimensions and the kinematics of parts. At the different levels of detailing, requirements for assembling, manufacturing, etc. are specified. The second pillar represents the drive unit (e.g. electric, pneumatic or hydraulic) with its supply unit. The third and last pillar is dedicated to measurement techniques.

At the mechatronic interconnecting level, all specific design parameters (e.g. type of drive, length of clamping lever, clamping and holding torque), describing the coupling between the different domains, are collected. The requirements of the mechatronic design problem are issues such as the desired clamping and holding forces. If – due to a new requirement – the clamping force should be controlled, we can simply extend the mechatronic pillar model with a domain-specific component for suitable controllers.

In order to clamp complex sheet metal parts, it is necessary to use several clamping devices. All of them represent mechatronic modules, which are combined through their positions on the parts. Naturally, it is impossible to produce a welded structure of good quality, in agreement with the geometrical tolerances for the welded assembly, if one or more of the clamping devices are displaced from their correct positions, or the geometric deviations of the incoming sheet metal parts are too high. This dilemma can be identified through detection of geometric deviations by measuring the clamping forces at each clamping device and evaluating them in an integrated software module.

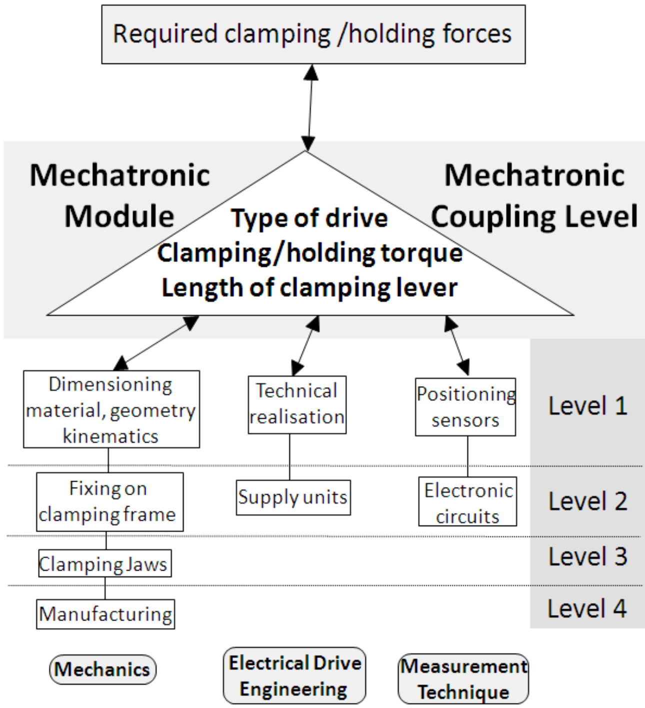

Figure 4.6: Application gripper: parameter hierarchy

5. CONCLUSION

In this contribution, the application of mechatronic system design principles is examined. As a result of this approach, two important advantages arise. Firstly, alternative, possible system structures may be established and evaluated and, secondly, it is possible to define a hierarchy of model parameters. Hierarchical models are very important tools to handle the increased complexity of such integrated design tasks. According to the increasing degree of detailing during the design process, the models become more and more detailed, leading to a hierarchy of models as well as their describing parameters. The author believes that this point especially has contributed a major portion to the success of modern mechatronic products on the market.

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CHAPTER 5

Mathematical Modelling as a Research Methodology

Zhongjie Huan

1. INTRODUCTION

Mathematical modelling is a process of creating a mathematical representation of some phenomenon in order to gain a better understanding of the expected functional characteristics and limitations of the phenomenon. It is a process that attempts to match observation with symbolic statement. During the process of building a mathematical model, the modeller will decide what factors (variables) are relevant to the problem and what factors can be de-emphasised – or even ignored – and can determine the relative effect of each input variable on the expected functioning (output) of the system under investigation. Once a model has been developed and used to answer questions about the phenomenon, it should be examined critically and, if necessary, modified to obtain a more accurate reflection of the observed reality. [1]

Thus, mathematical modelling is an evolutionary process and as new insight into the problem is gained, the process is optimised. The success of a model is determined by the ease of its use and the accuracy of its predictions.

With the development of powerful computer technology and numerical simulation technology, mathematical modelling is increasingly being applied to a wide spectrum of areas, not only in the areas of natural science, technology and engineering, but also in the areas of society, humanity, economics, and management.

For example, a biscuit company may wish to increase the throughput at a distribution depot. [2] Suppose the biscuits arrive at the depot on large articulated trucks, are unloaded, and transferred onto storage racks by fork trucks. When required, the biscuits are removed from the racks and loaded onto small delivery vans for dispatch to particular retail customers. To increase the throughput, a number of options might present themselves to the management. These include:

- increasing the number of loading or unloading bays;
- increasing the number of fork trucks; and
- using new systems for handling the goods; etc.

It would be possible to experiment on the real depot by varying some of these factors and evaluating the outcomes, but such trials would be expensive and time consuming.

The simulation approach to those problems involves the development of a model of the depot. The model is simply an unambiguous statement of the way in which the various components of the system (for example fork trucks and loading bays) interact to produce the behaviour of the system. Once the model has been translated into a computer programme, the high speed of the computer allows a simulation of, say, six months, in a few moments. The simulation could also be repeated with the various factors at different levels to see the effect of more loading bays, for example. In this way, the programmed model is used as the basis for experimentation. By doing so, many more options can be examined than would be possible in the real depot, and any disruption is avoided.

2. FEATURES OF MATHEMATICAL MODELLING

Compared to experimental research, mathematical modelling has the following characteristics:

2.1 Time saving

Admittedly, depending on the complexity of the system under investigation, mathematical modelling may require a significant amount of time to convert the practical project into an abstract mathematical model and to produce working computer programmes for simulation models. However, once these have been written, an attractive opportunity presents itself, namely, that it is possible to simulate weeks, months or even years in seconds of computer time. Hence, a whole range of possible alternatives may be properly compared simply by varying the appropriate variables.

2.2 Cost saving

Though simulation can be time consuming, and therefore expensive in terms of skilled manpower, real experiments may turn out to be even more expensive – particularly if something goes wrong! Experience shows that the cost of mathematical modelling is invariably and substantially cheaper than an experimental procedure of a similar value to the researcher. With the development of increasingly powerful computers with high data processing speeds, this cost-saving feature is even more evident and attractive.

2.3 Sufficient information

It is often difficult, or even impossible, to obtain specific, important information from physical experiments. In such cases, simulation of the system may prove to be the best way to access the necessary information. For example, suppose a metal rotor with the diameter of 200 mm rotates at the speed of 78000 RPM. Since it would be impossible to measure the airflow in the rotor and the rotor's temperature distribution experimentally due to the high speed, the only way to determine them would be by means of mathematical simulation.

Another example for consideration is in terms of spin casting. Suppose the time taken for the casting material to pass the solidification (melting) point is required. While it is impossible to measure this phenomenon, it is possible to mathematically model it.

2.4 Prediction

Mathematical models are being used widely to predict incidents as a function of time. Examples of successful predictions based on mathematical principles are, the weather forecast and disaster predictions such as hurricanes, tsunamis and typhoons. Prediction by means of mathematical modelling is often used to save lives and prevent human suffering. It can also be used in economics, finance, management and social science – such as for the prediction of economic growth and stock analysis and prediction.

2.5 Intuitive result display

Mathematical modelling can provide immense quantities of data that can be used for analysis. Such data may include 3-dimensional spatial coordinates and the relevant time coordinates. Consequently, intuitive (visual) results can be obtained to ease an understanding of the nature of the project (see Figure 5.1).

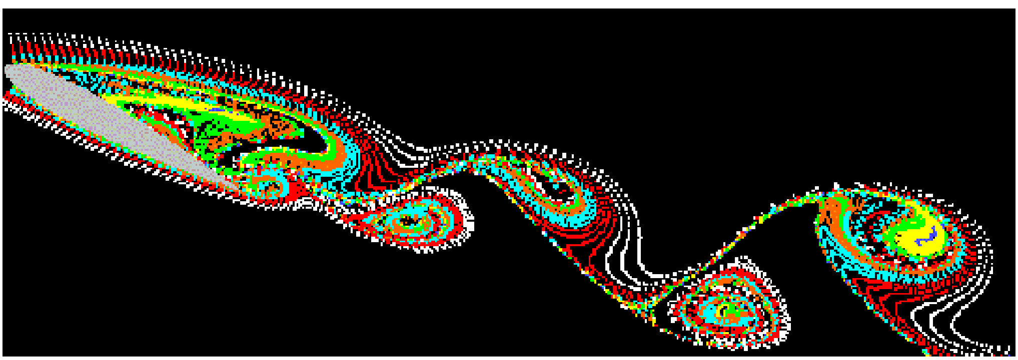


Figure 5.1: Streamlines of unsteady flow about a two-dimensional airfoil [4]

For transient problems, an animation of the results is also possible for investigation.

2.6 Replication

Unfortunately, in the experimental world, it is rarely possible to exactly produce a precise replication of an experiment. One of the important skills of physical scientists is the design of experiments which are repeatable by other scientists. However, in some disciplines, this is rarely possible. For example, it seems unlikely that an organisation's competitors will sit idly by whilst a variety of pricing policies are attempted in a bid to find the best. It is even less likely that a military adversary will allow a replay of a battle. In contrast, mathematical modelling is exactly repeatable.

2.7 Safety

One of the objectives of a simulation study may be to estimate the effect of extreme conditions, and to do this in real life may be dangerous or even illegal. It might not be permitted to carry out an experimental nuclear explosion and thus, modelling may be the only feasible way to study such dangerous events. Similarly, even though it is often impossible to physically study real hurricanes, tsunamis and typhoons, mathematical modelling of such phenomena can be carried out safely.

3. PROCEDURE OF MATHEMATICAL MODELLING

Mathematical modelling is the process of creating a mathematical representation of a phenomenon. It is a process that attempts to match observation with symbolic statement or a bridge linking the physical world with the mathematical world.

Mathematical modelling entails the following two components, namely physical issues and mathematical issues (see Figure 5.2):

- The physical issue is to establish the physical model based on a practical problem and the research targets, and to derive the new practical knowledge from the mathematical results through analysis.
- The mathematical issue includes the establishment of the mathematical model based on the established physical model – normally expressed as equation sets – and solving the mathematical equations to obtain the mathematical results.

The mathematical modelling procedure is shown in Figure 5.3.

The process starts with an analysis of a practical problem. At this stage of the study, some assumptions and simplifications have to be made to simplify the practical problem, after which the physical model can be defined mathematically. This is an important stage with an impact on the accuracy of the model.

Based on the physical model, the mathematical model can be written in the form of mathematical equation(s), which have to be solved using mathematical methods.

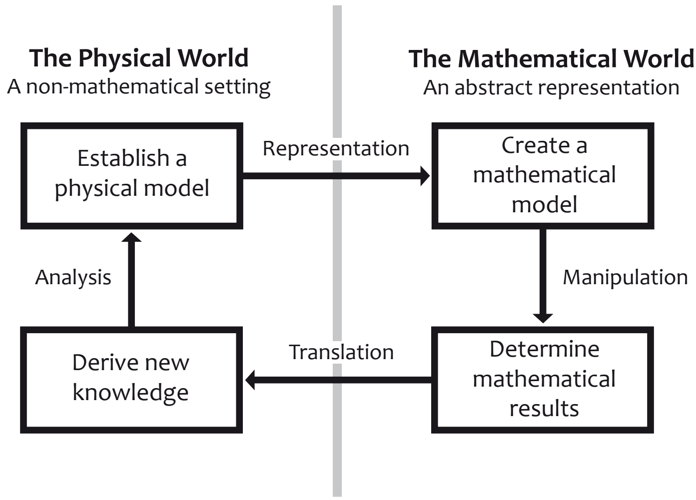


Figure 5.2: The principles of mathematical modelling

The next critical step is the verification of the correctness of the model. Only a model reflecting the true status of the phenomenon should be used for further analysis. It is often not possible to numerically verify the accuracy of the results. Thus, the previous knowledge, intuition and experience of the modeller are normally very important during this phase of the research.

Mathematical modelling normally is an evolving or iterative process. The initial model is refined by sequential mathematical processes and careful evaluation of the results obtained. Thus, it is conceivable that some physical processes can never be solved exactly and refinement of their models might be carried out over several generations of researchers.

4. SPECIFIC ISSUES OF MATHEMATICAL MODELLING

Building a mathematical model for your project can be a challenging, yet interesting, task. A thorough understanding of the underlying scientific concepts is required.

Although different problems may require very different methods of modelling, the following issues are always important.

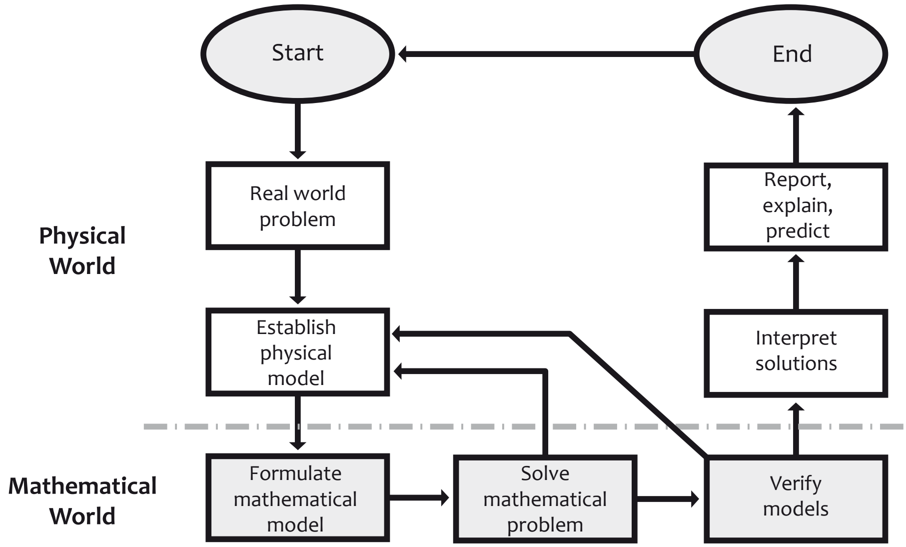


Figure 5.3: The modelling procedure

4.1 Establishment of the physical model

1. *Identifying the problem*

The terms of the problem are defined and diagrams drawn where appropriate. For example, when a dynamic thermo fluid problem is to be solved, general concerns of the problem include the pressure distribution, temperature distribution, flow velocity of the fluid, etc. Factors influencing the system, such as the kinds of fluid, the compressibility of the fluids, the viscosity of the fluid, the state of liquid, the geometry of the objects, steady or unsteady state, etc. should also be considered.

During the analysis, the target function or the output variables and the influencing factors must be identified. For example, when the cooling process of spin-casting manufacture is investigated, heat transfer characteristics and fluid mechanics are to be considered. Factors influencing the process include the mould halves, the casting material and temperature, the flow of the material in the cavity, the contact thermal resistance between the two halves, the rotation of the mould and the environmental conditions. The temperature distribution and solidification process of the part in the mould is to be determined.

2. *Simplification of the problem (physical model)*

It is usually good to begin with a simple model and to state the assumptions that are made whilst focusing on particular aspects of the phenomenon.

Any assumptions may cause errors in the result obtained for the problem. Thus, absolutely accurate results can be expected only in the case of no assumptions in the definition of the mathematical description of the problem. However, in practice, due to the complexity of physical systems, it is usually impossible to obtain exact results using modelling, whilst a fair approximation of the system is acceptable for modelling purposes. Thus, reasonable assumptions are usually acceptable.

General assumptions and simplifications include:

A. State assumption: from transient problem to steady state problem

Strictly speaking, no process and state are in a steady state, but in order to simplify the analysis, some states can be regarded as steady. Examples of systems that are considered as being in a steady state are a normal functioning cold store or air conditioning system, and a vehicle travelling at a constant speed.

Such assumptions are also dependent on the context of the investigation. For example, whilst studying the production process of a plastic injection moulding machine, if you are concerned about the micro process from the moment of filling of the mould with molten plastic to the eventual delivery of the final solidified product, the process of one shot cannot be regarded as steady – it is time-dependent. However, if your attention is the long-term operational features of the complete production line, the same activity can be regarded as a steady state process.

B. Geometry assumption: from three-dimensional to two-dimensional or one-dimensional

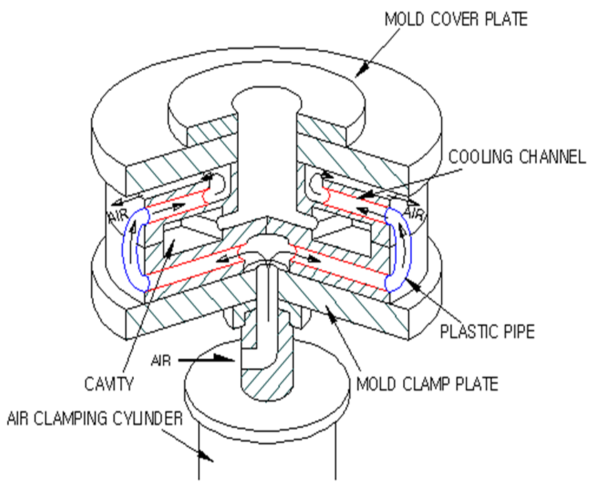
All physical objects are three-dimensional (3-D) in shape, but in most cases they can be simplified to be represented as a 2-D or 1-D model, whilst retaining high accuracy in the prediction of the operating parameters thereof.

For example, a long, thin rod can be simplified as a 1-D model, whilst a thin plate can be regarded as an equivalent 2-D or even 1-D model. Similarly, axial-asymmetrical objects, like a rotating cylinder, can be regarded as 2-D problems. Figure 5.4 shows a 3-D spin-casting model, simplified to a 2-D model.

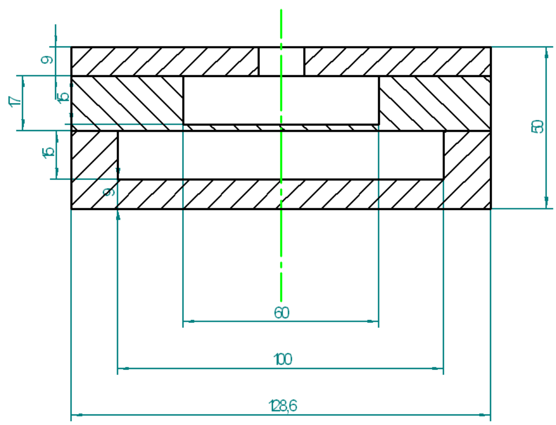
C. Physical assumption: Ignore unimportant factors pertaining to the problem

During mathematical modelling, some unimportant factors can be ignored in order to simplify the modelling process. For example, in the cooling process of spin-casting, the factors influencing the heat transfer of the part and mould include:

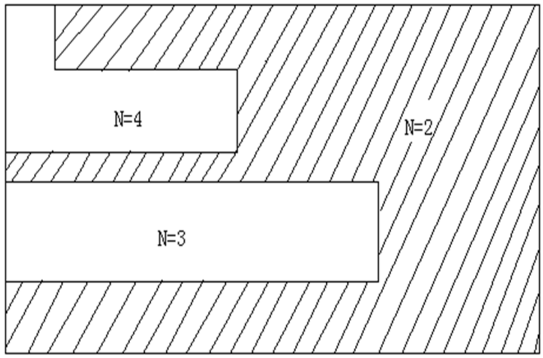
- conduction heat transfer of the mould,
- conduction heat transfer of the part after the solidification,
- phase change process of the casting material,



(a) 3-Dimensional original spin-casting machine set-up



(b) Full-sized simplified 2-Dimensional model



(c) Half-sized simplified 2-Dimensional model

Figure 5.4: Demonstration of geometry simplification [5]

- flow of the casting material (the filling of the mould with the material),
- convection heat transfer in the liquefied material,
- contact heat transfer between the casting material and the cavity,
- contact heat transfer between the mould halves,
- convection heat transfer of the mould surface,
- radiation heat transfer between the mould surface and the environment,
- airflow of the surrounding space, etc.

This is obviously a complicated phenomenon which is hardly possible to solve taking into account all the above characteristics. In practice, however, several of these variables are negligible. Consequently, the flow of the material, the convection heat transfer of the liquefied material, the contact heat transfer between the material and the cavity as well as between the mould halves, the radiation heat transfer, and the airflow of the surrounding space can all be ignored without seriously compromising the accuracy of the resultant mathematical model.

D. Specific simplification of the physical properties

Sometimes, in order to simplify the mathematical model and to solve the model easily, some physical properties need to be simplified in a specific way.

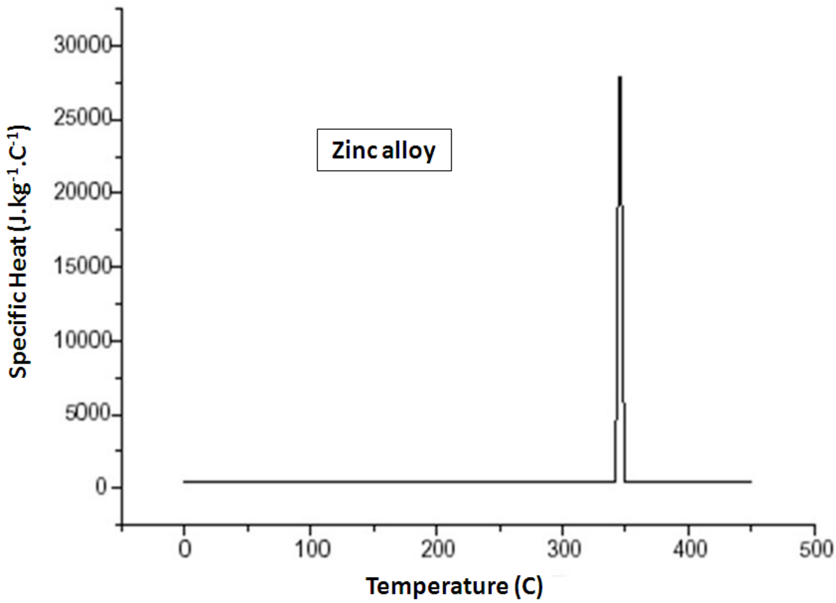


Figure 5.5: The conversion of latent heat to specific heat [5]

For example, the latent heat dissipated during the phase change, as in the above-mentioned example, can be regarded as a part of the specific heat (Figure 5.5), then the governing equation can be converted from

$$\rho C \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + q(T)$$

to

$$\rho C(T) \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T)$$

and, consequently, the computer programme used for the simulation will be much simpler.

4.2 Establishment of a mathematical model

Identify important variables and constants or parameters

Mathematical models typically contain three distinct types of quantities: input variables, output variables and parameters (constants). Output variables represent the model solution. The choice of what to specify as input variables and what to specify as parameters is somewhat arbitrary and often model-dependent. Each input variable characterises a single physical problem while parameters determine the context or setting of the physical problem.

For example, in modelling the decay of a radioactive material, the initial amount of material and the time interval allowed for decay could be input variables, while the decay constant for the material could be a parameter. The output variable for this model is the amount of material remaining after the specified time interval.

Continuous-in-time vs. discrete-in-time models

Mathematical models of time-dependent processes can be split into two categories depending on how the time variable is to be treated. A *continuous-in-time* mathematical model is based on a set of equations that are valid for any value of the time variable. The solution of a continuous-in-time mathematical model provides information about the physical phenomenon at every possible time value.

A *discrete-in-time* mathematical model is designed to provide information about the state of the physical system only at a selected set of distinct times. The solution of a discrete-in-time mathematical model provides information about the physical system at a finite number of time values only.

Continuous-in-time models have two advantages over discrete-in-time models:

- They provide information at all times, and
- They show the qualitative effects that can be expected when a parameter or an input variable is changed more clearly.

On the other hand, discrete-in-time models have two advantages over continuous-in-time models:

- They are less demanding with respect to the required skills levels in algebra, trigonometry, calculus, differential equations, etc., and
- They are better suited for implementation on a computer.

Develop the equation(s) that expresses the relationships between the variables and constants

In this process, which is often the most demanding of the entire modelling process, the natural laws are normally used to relate the variables, constants and properties.

4.3 Solving the mathematical model

Generally, there are three methods of solving the equations as defined:

Exact solution

Some equation(s) can be solved analytically and an exact solution can be obtained. These kinds of solutions are mostly found not to be very accurate when applied in practice, although they are clear and the researchers find it easy to understand the modelled phenomenon. The results are continuous.

Semi-exact simulation

Some mathematical equations can be solved by a combination of analytical and numerical methods. In this case, the output variables can be expressed as mathematical equations which are still difficult to understand. They can usually not be directly applied to the application, and exact results can only be obtained by virtue of numerical techniques. The results are discrete.

Numerical simulation

For most engineering projects, numerical methods are required to obtain discrete solutions.

Numerical methods generally adopted are Finite Differential Methods (FDM), Finite Element Methods (FEM) and Boundary Element Methods (BEM). Different methods have different features and are used in different applications. It is easy to use FDM to discretise the equations but this is not suitable for complicated geometry and non-linear problems, whilst FEM is suitable for complicated geometrical boundary and non-linear problems.

In the mathematical representation of a physical phenomenon, some assumptions are applied to the physical model. Sometimes, further simplification is required during the solution of the mathematical equations. For example, the order of magnitude for different terms of equations can be used to neglect some unimportant terms in order to simplify the equations.

The selective laser sintering (SLS) melting process [3] may be taken as an example where, before melting, there are gases in the pore space between particles of the powder to be sintered. It is straightforward to express the density and heat capacity of the unsintered powder bed as:

$$\rho_s = (1 - \varepsilon_s)\rho p + \varepsilon_s \rho_g$$

$$(\rho c_p)_s = (1 - \varepsilon_s)(\rho c_p)_p + \varepsilon_s (\rho c_p)_g$$

where ρ and (ρc_p) are the density and heat capacity respectively, the subscripts p and g denote particle and gases. ε_s is the volume fraction of the gases in the unsintered power bed. This coincides with porosity for the unsintered bed, i.e. $\varepsilon_s = \frac{V_g}{V_g + V_s}$, where V_g and V_s and are the volumes of gases and solid particles.

The order of magnitude of the typical metal powder and gas thermal properties are as follows:

$\rho_s \sim 10^3 kgm^{-3}$, $(c_p)_s \sim 10^2 Jkg^{-1}K^{-1}$

$\rho_g \sim 1 kgm^{-3}$, $(c_p)_s \sim 1 Jkg^{-1}K^{-1}$

Thus, the contribution of gases to the density and heat capacity of the powder bed is negligible. The thermal properties of the powder bed before sintering can, therefore, be expressed as:

$$\rho_s = (1 - \varepsilon_s)\rho_p$$

$$(\rho_c p)_s = (1 - \varepsilon_s)(\rho c_p)_p$$

4.4 Verification of the model

Once the model has been developed and applied to the problem, the resultant solution must be analysed and interpreted with respect to the problem. The interpretations and conclusions should be checked for accuracy by asking the following questions:

- Is the information produced reasonable?
- Are the assumptions made while developing the model reasonable?
- Are there any factors that were not considered that could affect the outcome substantially?
- How do the results compare with real data, if available?

In answering these questions, it may be needed to modify the model. This refining process should continue until a model is obtained that agrees as closely as possible with the real world observations of the phenomenon that is modelled.

There are three practical approaches to verify the accuracy of mathematical modelling.

Verification by the extreme case

The model can be narrowed to the case of an extreme condition, and its value can be verified by the results.

For example, the dimensionless solid-liquid interface location with time in the SLS process [3] can be deduced as:

$$\frac{dS}{d\tau} = \frac{1}{1-\varepsilon_s} erfc\left(\frac{(1-\varepsilon_s)S}{2(1-\varepsilon_l)\sqrt{(\tau-\tau_m)}} \right) - \frac{2K_S Sc}{\Delta - S}$$

Where S and τ are the non-dimensional interface location and time, ε is the volume fraction of the gases or liquids in the unsintered power bed; subscripts s and l denote solid and liquid; K_S, Sc, and Δ are constant parameters.

It should be noted that if $\varepsilon_S = \varepsilon_l = Sc = 0$, the equation above is reduced to

$$\frac{dS}{d\tau} = erfc\left(\frac{S}{2\sqrt{\tau}} \right)$$

which is identical to the proven result of El-Genk and Cronenberg [7].

Verification by basic governing principles

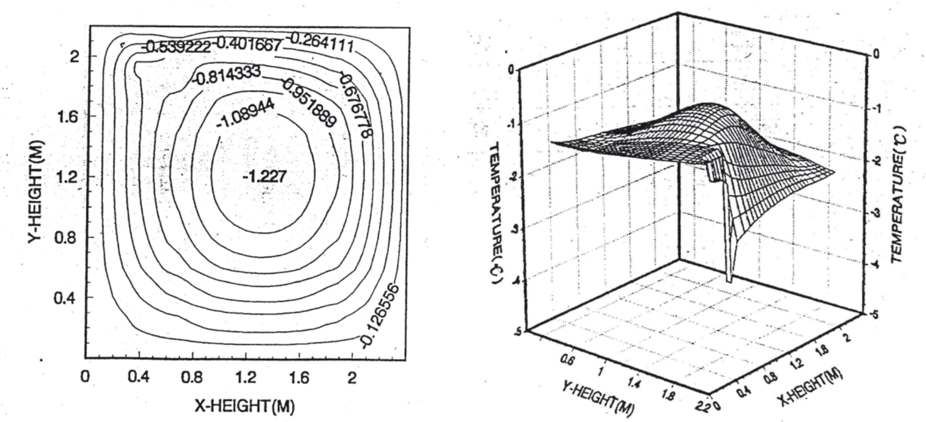
Reasonable assumptions and simplifications made during the modelling process must not violate any laws of nature, and the basic governing principles must be observed. Examples of important natural laws are the conservation of mass, momentum and energy.

Once the modelling results have been obtained, it must be investigated whether the results violate any natural laws or not. If the results are in contradiction with any of the natural laws, a vital error must have been made during the modelling. Errors must be identified as such and corrected, no matter how promising the results appear to be.

A situation is described in [8] where the simulation of a particular phenomenon resulted in invalid results. The 3-dimensional airflow and temperature field of a compact cold storage facility was simulated numerically. It was assumed that there was a steady state of airflow and a non-sliding flow over insulating bodies; the outlet of the cooler was set as the first condition for the airflow field. The store was assumed to be empty.

One of the simulated results is shown in Figure 5.6, in which the temperature with negative values is reasonable and the curves and figures look beautiful.

However, from the simulation results, it is obvious that the temperature in the central area is higher than that of the surrounding areas, which means that there is a temperature gradient to the outside. This implies that heat flows from the central area to the surrounding areas, and it is obvious that there must be a heat source in the central area.



Streamline in the cold storage Temperature distribution in the cold storage

Figure 5.6: Incorrect simulated results of the airflow in a cold storage

However, according to the assumption the cold storage is empty and a steady state is assumed. That means there is no heat generation in the cold storage.

Consequently, the simulation result is in conflict with the physical model and the simulation is wrong. Thus, it is not necessary to review any other results and in conclusion, the results are, beyond any doubt, unreliable.

Experimental verification

Experimental verification is the general – and often preferred – method to confirm a mathematical model. Of course not all the simulated results can be tested but some experimental results, which are important and feasible to obtain, are used to verify the simulation model under identical conditions. If the simulated results approach the experimental results to an acceptable degree, the mathematical model would not be accepted as proven wrong – even if, also, we cannot say the modelling is perfect.

For example [5], zinc alloy was used as casting material to verify simulation results for the spin-casting process. The mould surface temperature and the bottom temperature at the central point were measured 10 minutes after the casting material (at a temperature of 420°C) was poured into the casting cavity. The measured temperature of the top surface at a point 1.8 cm from the central point, were in the range of 62-68°C, whilst the calculated result was 67.2°C. A typical temperature of the bottom surface of the casting part at the central point was measured as 268.7°C, with a calculated value of 274.6°C. Therefore, in both instances, the calculated values corresponded well with the experimental results (see Table 5.1) and the model was regarded as a valid approximation of the experimental situation.

Table 5.1: Comparison between measured and calculated values [5]

	Temperature on top surface	**Temperature on bottom surface**
Measured values	62.0-68.0°C	268.9°C
Calculated values	67.2°C	274.6°C
Relative error	1.2-8.4%	2.2%

Another example is an experimental verification of computational results for the freezing process of quick-frozen foods.

The freezing process of a slab of beef with a thickness of 40 mm was measured and calculated (Figure 5.7) [9]. The experimental freezing time was 3.57 hours from an initial temperature of 15°C to the final central temperature of -15°C, whilst the calculated result was 3.88 hours. The freezing curve from the calculated results agrees closely with the curve from the experimental results, and the model could be accepted as reliable.

After the verification of the mathematical model, the simulation can be carried out under different conditions and, consequently, new knowledge can be derived from the numerical results.

5. CONCLUSION

Mathematical modelling, as an important research approach, is applied widely in research. With modelling, practical projects are converted into pure mathematical problems. During the conversion process, the physical model must be described as mathematical equations, based on the physical model and natural laws, as well as on reasonable assumptions and simplifications.

After the relevant equations have been solved, the accuracy of the models must be verified before the models can be applied to practices in a wider range.

Mathematical modelling cannot be completed in one cycle, but models normally need to be refined in subsequent cycles of refinement.

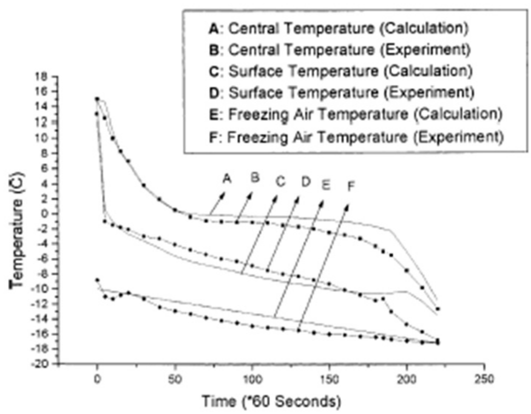


Figure 5.7: Experimental verification of the modelling of quick-frozen foods

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CHAPTER 6

Physical Modelling of Terrains and Structures

Sanat Agrawal and Gerrit Jordaan

1. USE OF SCALE MODELLING

Physical models are normally used in any of the following circumstances:

- When no, or only extremely complex, mathematical equations are available by means of which analytical solutions of the system under investigation can be obtained;
- When physical structures with very complex geometries are to be studied;
- If any structure is to be exposed to very complex external stimulations.

Examples of situations that lend themselves to physical modelling are:

- offshore structures;
- turbine blades;
- rocket engines;
- jet airliners and missiles; and
- hydraulic transmission.

The expected performance of a system may be required in unattainable situations – e.g. prohibitive size or expense, unfriendly environments, high speeds or dangerous situations – in which case physical modelling may be the only way in which it may be possible to acquire the required information.

Current design philosophy of structures necessitates seismic testing of structures using pseudo-dynamic tests in those cases where forces and displacements to which structures are expected to be exposed are large. Typically, due to limitations of the testing equipment and the costs involved, such tests are likely to be executed by means of scaled models.

As the complexity of a system under development increases, the designer's confidence in its theoretical design would decrease, and physical modelling would typically be used to verify the accuracy of design formulae or mathematical models used to study the expected performance of the system. This would increase confidence in the design and may impact on the eventual decision on whether to proceed with the construction of the actual prototype.

2. HISTORY OF SCALE MODELLING

The use of scale models is almost as old as engineering itself. It is known that even Galileo was aware of many important criteria and limitations of scale models. However, it became a well-respected scientific discipline during the mid-nineteenth century with the upsurge in engineering-related problems – especially with reference to the increasing use of trains and increasing levels of industrialisation.

During this time, there was growing concern in the minds of some designers of bridges and other structures regarding the safety of their designs. This situation largely came to a head as a consequence of a bridge near the English town of Chester that broke on 24 May 1847, with a resultant loss of life. This caused unease about the continued satisfactory functioning of cast iron bridges and a renewed effort was made to quantify and optimise the practice of scale-modelling. In particular, the effect of vibration on such structures was studied – with mixed success.

This led to serious efforts by, *inter alia*, Eaton Hodgkinson, to accurately physically model the cast-iron Britannia train bridge. It was modelled to a length of four feet and with a dynamic load of less than 3kg. However, initially some experts said that the modelling was "...of little value on account of their having been tried on too small a scale".

G P Bidder, a well-known railway engineer of the time, believed the effect of vibration "...to be a mere ghost raised by mathematicians to frighten engineers as to strengthen their structures", whilst it has since been proven as a most important loading characteristic of any structure.

The even more sceptical Scott Russell said the following about a series of efforts to render scale modelling as a science:

"You will have on the small scale a series of beautiful, interesting little experiments, which I am sure will afford you infinite pleasure in making them, and will afford you infinite pleasure in the hearing of them; but which are quite remote from any practical results upon the large scale."

Subsequently, accuracies in the predicted performance of structures of between 0.2% and 19% were attained, and eventually this research resulted in a clear demonstration that scale models could be used to predict prototype behaviour on a systematic basis, and it became common practice.

3. WIND AND WATER TUNNELS

Aerodynamics plays a vital role in many fields of engineering. Testing of the aerodynamic characteristics of a system can take place in wind or water tunnels, depending on the available facilities and the information required. It is used to examine the streamlines and to determine the behaviour of aerodynamic forces on the model, and enables the modelling of new shapes in controlled environments.

4. SCALE MODELLING OF PHYSICAL STRUCTURES

Scale modelling is frequently used to investigate the expected operation of physical structures if they should be exposed to specified external loading. Of particular interest are those cases where artefacts are expected to move at a relatively high velocity through a medium such as air or water. In these cases, it is common to model this operation in wind or water tunnels.

It is often difficult to model particular phenomena accurately using mathematical techniques. It is then common to revert to the development of a physical model representing the system under investigation and to measure the effect of the expected external stimulation impacting on the system – utilising suitable instrumentation built into the model. Such measurements are subsequently scaled in terms of the design parameters of the physical model.

However, if possible, the modeller would try and verify the validity of those elements of the scale model for which mathematical modelling is a viable proposition. In this manner, the value of the model is dramatically increased, with a resultant increase in the confidence level of the designer. For example, computational fluid simulation techniques can be utilised to derive the expected performance of a model under particular conditions, in order to ascertain the validity of measurements made during testing with the relevant scale model.

Similarly, mathematical analysis of wind tunnel data is used during the evaluation of results obtained whilst testing a physical model.

A tunnel in this context consists of:

- a contoured duct to control direct fluid flow,
- a drive system to move a fluid,
- a model to be tested, and
- instrumentation to measure forces on the model.

The use of such tunnels is very common and used extensively to determine the quantifiable parameters of the scale model. Velocity, time, stress, force and power are typical examples of parameters that are normally measured. To enable an accurate prediction of the expected functional behaviour of the prototype, these values are then scaled in proportion to the relative size of the model compared to that of the prototype (see paragraph 5.1).

The development and scale modelling of modern, high-speed aircraft and missiles often necessitates that such testing be done in wind tunnels with extremely fast airflows. Thus, the use of wind tunnels with even supersonic wind speeds is no longer the exception, but common practice.

4.1 System simplification in physical modelling

The development of a successful model requires knowledge of the system to be modelled, including the relevant variables, interactions and dynamic behaviour of the different elements. Considering these, the optimum model is developed by consideration of the model validity – in terms of measurability, accuracy, repeatability and executability. If possible, the accuracy of collected data is normally verified against measurements taken on the actual system.

As with mathematical modelling, scale models are often designed to simulate only particular characteristics of the prototype, such as vibration, heat-transfer, wind resistance, etc. In the interests of cost-saving, often only the most essential features are modelled. Minute details of a design are often not critical to the functioning of the prototype and are not modelled in such cases.

4.2 Physical modelling of the effect of water and waves

From the middle of the nineteenth century, physical scale modelling was used extensively to study the expected behaviour of boats whilst afloat. In particular, the resistance of a ship to the flow of water against its sides at different speeds, and its expected rolling in the water, have been studied extensively using physical models. The rolling of a ship is often studied as a function of the ship's isochronism with the waves that the prototype is expected to encounter. For this, a controllable wave-maker and a suitable model of the ship are used.

Even though substantial resistance was experienced initially, with regard to scale modelling of ships, clear evidence was gradually gathered to demonstrate that scale models could be used to predict the behaviour of ships on a systematic basis. Very specific formulae were developed over a period of time to interpret results obtained in this manner.

The use of hydrodynamic scaled models of offshore structures is often used to verify numerical or analytical predictions of global and local hydrodynamic loads on the prototype. In this manner, the effect of wave loading on these models is studied. Examples of global loads are shear and overturning moment at the base of the structure, whilst local loads include wave impact and run-up. These phenomena are usually modelled using relatively large scale models (for example, 1:40).

Particular constraints of such structures are their geometry (related to the hydrodynamic scaling of the model), load measurement accuracy over a specified range, and specific wave parameters. The models are usually mounted in a suitable wave basin.

Such systems normally meet specified criteria, such as:

- water depth,

- ranges of wave heights and periods, as well as wave spectra of irregular waves,
- the dimensions of the model, and
- the hydrodynamic scale.

5. SIMILARITY LAWS IN MODEL TESTING

To predict the actual behaviour of the prototype with measurements made on a scale model, there must be similitude between the model and the prototype. Similitude is used to establish a set of scaling factors between the model and the prototype. The most important types of similitude are geometric, kinematic and dynamic.

5.1 Geometric similarity

The model and prototype are assumed to be geometrically similar only if all the pairs of points on the model and prototype have the same ratio of distances in all three coordinates. Thus, there is a fixed, linear relationship between the relative positions on the model and prototype. This is called the (length) scale factor. For models satisfying this characteristic, the value of any parameter measured at any point with respect to the model is related to the value at the homologous point (i.e. a point having the same location relative to the prototype) through the corresponding scale factor.

However, it is often impossible or not feasible to scale a system by the same margin in all coordinates. This practice is particularly common in the study of geographic structures, dams, etc. This requires particular expertise in assessing any measured values.

5.2 Kinematic similarity

The motions of the model and prototype are kinematically the same, if the relative velocities in the flow fields are the same. An example of this would be that the ratio of wind speed to revolutions per minute of a windmill, or wind-powered electrical power generating system, should be the same for the model as for the prototype, to enable effective transfer of data from the model to the prototype.

5.3 Dynamic similarity

This requires geometric similarity and ensures kinematic similarity between the model and the prototype. It occurs when the prototype and model force and pressure coefficients are identical. It usually requires a tenfold increase in the speed of the fluid to evaluate a model, one-tenth the size of the prototype.

6. PHYSICAL MODELS OF TERRAINS

Scale modelling is a term primarily used in Fluid Mechanics. Dimensions and other physical variables are scaled as required. However, the dimensions along the three coordinate axes are normally scaled uniformly. To ensure geometric similarity, the ratios of all corresponding dimensions in the model and prototype are equal.

However, there are applications where the dimensions are scaled non-uniformly as well. For example, the physical models of terrains are sometimes made with a non-uniform scale. This is different from typical scale modelling in mechanical engineering. Terrain models are given non-uniform scales for better visualisation of features. A physical model of a terrain is a very effective communication tool. It helps in studying possible dam structures and in improving insight into the expected terrain to be flooded if a prospective new dam fills. Similarly, it can be exceptionally useful for the design of roads in mountainous areas.

The following are examples of terrain models, prepared using digital elevation model (DEM) data. The data, obtained from a GIS vendor, was converted into .STL files and fabricated using a laser sintering process.

Figure 6.1 shows a schematic diagram of Table Mountain, as seen from the south-east – with the coast shown furthest in the figure. This diagram was derived from geographic data.

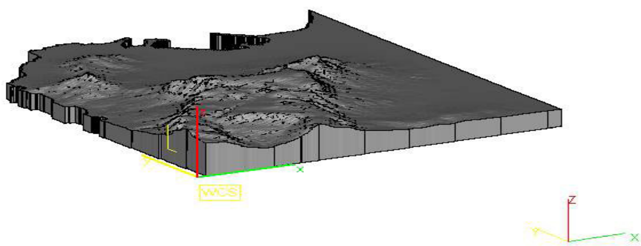


Figure 6.1: Table Mountain from the south-east

A physical model was subsequently built with polyamide (nylon) using a Laser Sintering (LS) process, resulting in a model as shown in Figure 6.2.

Figure 6.2: A polyamide model of Table Mountain as seen from the north-west

Figure 6.3 represents a scale model of an area of the Modder River sub-catchment. However, as is obvious from the figure, use of a uniform scale in all dimensions sometimes renders models with little or no practical value. Thus, it is common to enhance the characteristics in the vertical direction by using a different scale in that direction.

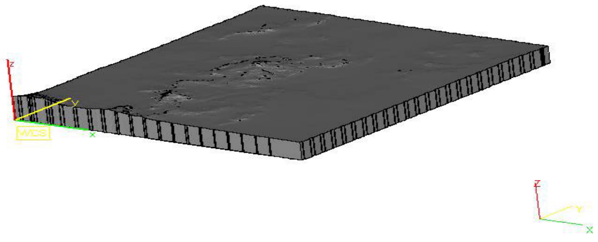


Figure 6.3: A region of the Modder River sub-catchment

This would result in a situation such as shown in Figure 6.4. Here the scales in the x and y-directions are equal to 1:45000 relative to the raw data, whilst a scale of 1:4500 is used in the z-direction. Thus, the elevation is given a scale of 10 relative to plan. Any changes in the vertical direction are now much more pronounced and their probable effects predictable. Considering that the regions shown in Figures 6.3 and 6.4 are quite similar, this practice created a huge difference between the two representations of the relevant areas – adding significant value to the model.

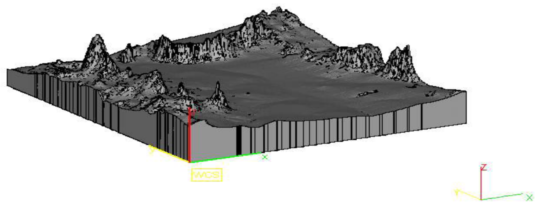


Figure 6.4: Another region of the Modder River sub-catchment (utm2628_32)

Obviously, in areas with large variations in the z-direction, differential scaling is often not required. An example of this is shown in Figure 6.5, where a physical model of the Amphitheatre in the Drakensberg Mountains is shown with a uniform scale. In this case, a uniform scale is a viable proposition since the terrain has a change in vertical height of over 300m over a very short distance.

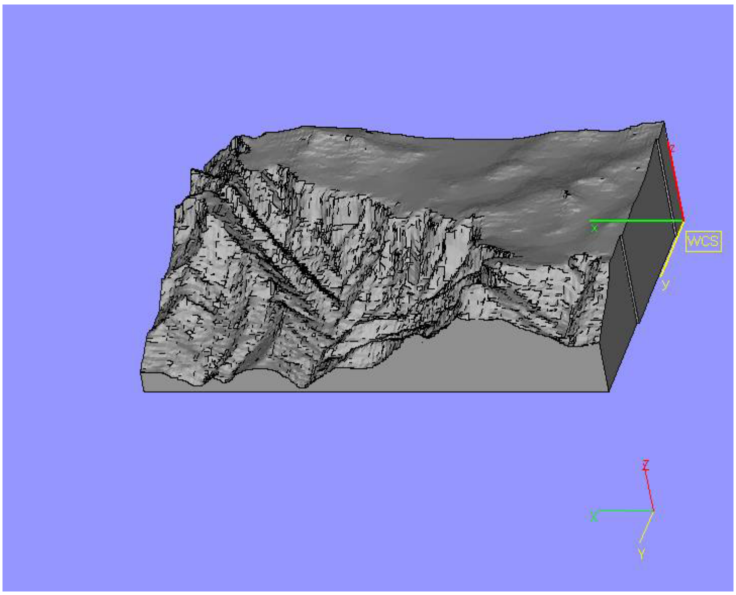


Figure 6.5: A model of the Amphitheatre with a uniform scale

7. MATERIALS USED IN THE CONSTRUCTION OF A SCALE MODEL

The materials used in a model are of particular importance and their functioning under the simulated conditions should approach that of the final material under normal operating conditions. This often necessitates the use of materials in the model of which the characteristics approach that of the ideal, but are not equal to it. An important example of this is the surface characteristics of the modelling material in a study of wind resistance and water flow, in the case of a model of a dam and its surrounding area.

8. SUMMARY

With the continuous development of new mathematical techniques, scale modelling has, to some extent, been superseded by mathematical modelling. However, it still forms an integral component of the normal design and development process used in modern engineering – and is expected to maintain its importance in the foreseeable future.

It is particularly valuable in contributing to a better understanding of the underlying principles governing the functioning of a system under investigation, as well as in improving the system designer's confidence in the design.

Scale modelling is a very complex field of study and this chapter is only an attempt at sensitising researchers to it as an important research and development methodology. It is inconceivable that any student of fluid mechanics would ignore the possible benefits that could be realised from using it, in trying to determine the expected performance of a new system under development, in verifying the accuracy of its design.

CHAPTER 7

Data Acquisition as a Research Procedure

Herman Vermaak

Objectivity is a fundamental prerequisite of scientific investigation. It is not easy, even for people with the best intentions, to interrogate a process and report data in an unbiased way, but this is a primary goal to which scientists should aspire. Skill at avoiding bias comes with experience, but depends mainly on understanding the goal of an investigation and carefully considering how to achieve it. Objectivity on the part of the researcher is a fundamental need for any data acquisition, interrogation and reporting process.

1. WHAT IS DATA ACQUISITION?

Data acquisition is the process of obtaining and recording primary experimental information. It involves collecting signals from measurement sources and (usually) digitising the signal for storage, analysis, and presentation on a personal computer – although dedicated data acquisition equipment is also available for this purpose.

Proper data acquisition and record keeping is an essential feature of experimental science and technology. It provides the foundation information on which subsequent data analysis and generalisations are based.

2. WHAT IS RECOGNISED AS DATA?

Data can belong to any of the following categories:

- *Quantitative*: Recorded numbers, graphs and charts of raw, numerical experimental results, and instrument output including photographs and digital images from which quantitative data can be derived.
- *Qualitative*: Notes of any type, some types of instrument output, photos, movies and digital images.
- *Original samples in unanalysed form*: e.g. biological specimens.
- *Research tools*: Protocols; computer software.

3. CLASSIFYING DATA

Data is classified according to the following framework:

- *Raw data*: Information obtained directly from experiments, surveys, etc. It includes information in laboratory notebooks and instrument output; may include information in computers.
- *Processed data*: Graphs, equations, tables, descriptions, summaries, and conclusions derived from raw data but not yet released to the public.
- *Published data*: Information distributed to people beyond those involved in the acquisition of the data and project administration. Theses and dissertations are published and become available to the public in a library.

4. A DATA ACQUISITION SYSTEM

Most modern industrial processing systems, factories, machinery, test facilities and vehicles, incorporate hardware components and computer software, the behaviour of which follows the laws of physics. Such systems often contain thousands of mechanical and electrical phenomena that are continuously changing; these phenomena are not in a steady state. The measurable quantities that represent the characteristics of a system are called variables. The proper functioning of a particular system depends on certain events taking place and the values of certain variables at a certain moment in time. When studying such a system, researchers are interested in the values of the variables, such as location, magnitude and speed, and use a variety of instruments to measure and record them. The variables are assigned units of measurement, such as volts, kilograms and metres per second, to name but a few.

Most variables must be measured with a device that converts the phenomena into a form that a human can perceive and interpret, such as a visual display, sound, or vibrations, to stimulate physical sensations. The conversion devices are called transducers or sensors, and they normally translate the physical phenomena to electrical signals (or vice versa) to be measured with electronic instruments. These instruments have traditionally been ammeters, voltmeters, and various other gauges, and the variables can be observed in real time. However, an increasing need (and the ability) to record and preserve these phenomena and analyse them at a later stage, has forced engineers to develop modern data acquisition systems.

4.1 System setup

The first step in any data acquisition experiment, after parameter identification, is to install and connect the required hardware and software to the system under observation. Hardware installation usually consists of plugging a board into a computer or installing measuring modules into an external chassis. Software installation consists of loading hardware drivers and application software onto a computer. After installation of the hardware and software, the sensors can be attached to the system being tested, whereafter the data acquisition hardware should be calibrated. Calibration consists of providing a series of known inputs to the system and recording the corresponding outputs. For most data acquisition devices, calibration can be easily accomplished with software provided by the vendor.

After the hardware has been set up and calibrated, data acquisition can commence. It is normal to anticipate that successful data acquisition will take place if the characteristics of the signal to be measured are fully understood by the operator of the measuring system. However, in a practical application, a sensor and its connections might be picking up unacceptable noise levels and may require shielding. Alternatively, it may be necessary to use the measuring system at a higher rate, or perhaps to add an anti-alias filter to remove unwanted frequency components. These effects act as obstacles to precise, accurate measurements and to overcome them, it may be necessary to experiment with different hardware and software configurations. In other words, multiple data acquisition trials may have to be run in order to ensure the optimal functioning of the data acquisition system.

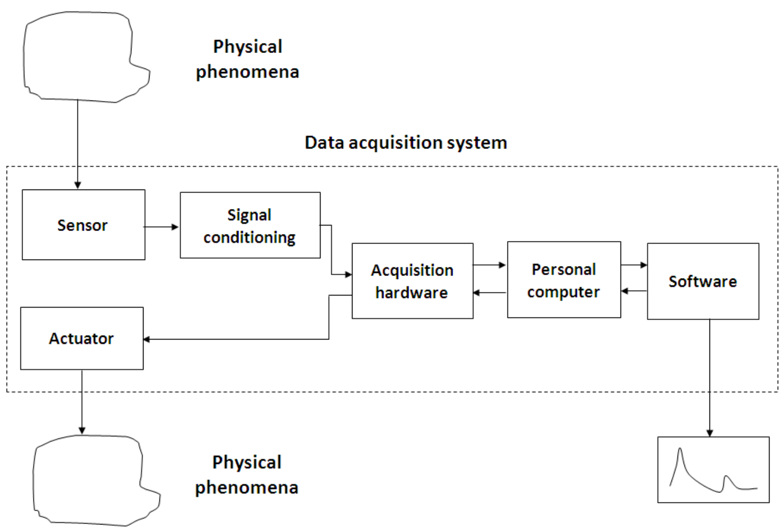


Figure 7.1: Basic configuration of a data acquisition system

Data is normally acquired by an analogue-to-digital converter (ADC) using a process called sampling. Sampling of an analogue signal involves taking a sample (determining the instantaneous value) of the signal at discrete times. The rate at which the signal is sampled is known as the sampling frequency. The process of sampling generates a series of values of the measured signal at definite time intervals, as shown in the following figures.

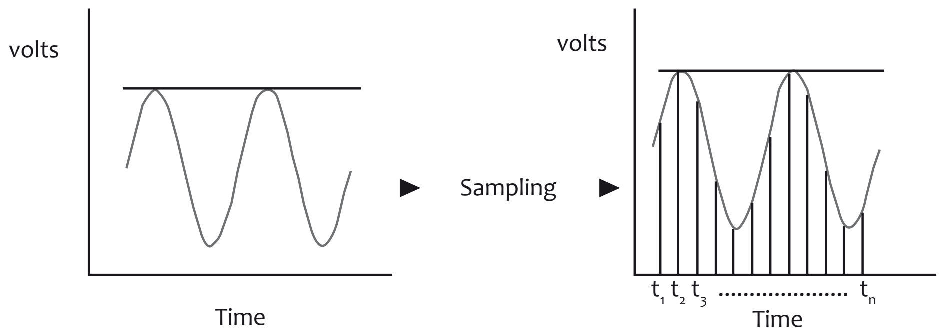


Figure 7.2: Process of sampling

The sampling frequency impacts on the quality of the converted analogue signal. Higher sampling frequencies normally achieve better conversion of the analogue signals. Conversely, the higher the sampling rate, the larger the amount of data, to be stored and processed for eventual interrogation of the accessed data, will be. However, the minimum sampling frequency required to represent the signal should be at least twice the maximum frequency of the analogue signal under test – this is called the Nyquist rate.

The resolution of the converted signal, and thus the precision with which the analogue signal is converted, is a function of the number of bits the ADC uses to represent the digital data. The higher the number of divisions the voltage range is broken into, the higher the resolution and, therefore, the smaller the detectable voltage changes. The resolution is an important characteristic of a data acquisition (DAQ) board.

The sampling frequency and resolution are very important factors in determining the performance of a DAQ system. Together with these factors, it is important to consider the environmental influences on the DAQ system. Susceptibility to electrical noise and extremes of ambient temperature, shock, and vibration are important characteristics of such a unit.

Most modern data acquisition systems will record extremely accurate, repeatable, reliable, and error-free data, provided the system is connected and operated according to recommended practices.

It must be noted that the quality of captured data is normally related to the operator's knowledge of the characteristics of the measured signals and the DAQ system utilised. Thus, there must be clarity of what is to be captured and, consequently, at what position in a system such a signal should be measured.

5. DAQ SYSTEM COMPONENTS

Data acquisition (DAQ) systems come in many different personal computer (PC) technology forms, offering great flexibility when selecting a particular system.

The following five components are to be considered when developing or selecting a basic DAQ system:

- Transducers and sensors
- Signals
- Signal conditioning
- DAQ hardware
- Driver and application software

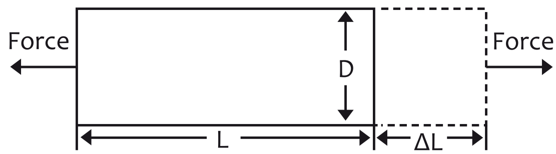
5.1 Transducers and sensors

A transducer is a device that converts a physical phenomenon into an equivalent, measurable electrical signal, such as voltage or current. The ability of a DAQ system to measure different phenomena largely depends on the transducers that are available to convert the physical phenomena into signals measurable by the DAQ hardware.

Table 7.1: Typical measured phenomena and transducers used

Phenomena	Transducer
Temperature	- Thermocouples - Resistive temperature devices - Thermistors
Light	- Vacuum tube - Photo sensors
Sound	- Microphones
Force and Pressure	- Strain gauges - Piezoelectric transducers
Position and displacement	- Potentiometers - Linear variable differential transformers - Optical Encoders
Fluid	- Head meters - Rotational Flow meters
pH	- pH Electrodes

An example of a physical characteristic to be assessed is the amount of strain on a body. Strain is the amount of deformation of a body caused by an applied force. More specifically, strain (e) is defined as the fractional change in length (see Figure 7.3).



$$\varepsilon = \frac{\Delta L}{L}$$

Figure 7.3: Strain on a body

While there are several methods of measuring strain, the most common is with a strain gauge, a device whose electrical resistance varies in proportion to the amount of strain in the device. The most widely used gauge is the bonded metallic strain gauge.

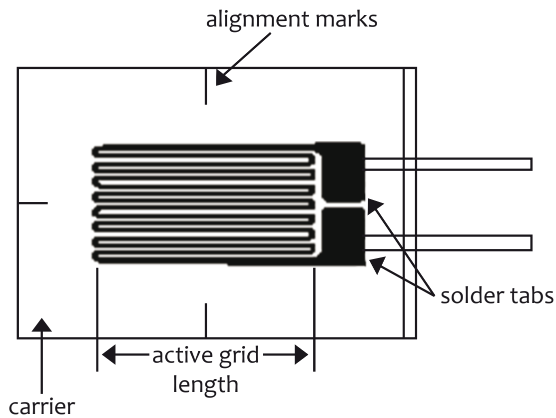


Figure 7.4: Physical parameters of a strain gauge

5.2 Signals

The transducer converts the relevant physical phenomena into measurable signals. Different signals need to be measured in different ways. For this reason, it is important to understand the different types of signals and their corresponding attributes. Signals can be categorised into two groups:

- Analogue
- Digital

5.3 Analogue signals

An analogue signal can assume any value with respect to time. A few examples of analogue characteristics include voltage, temperature, pressure, sound level and load. These characteristics are then converted by a transducer into an equivalent electrical signal. The three primary characteristics of an analogue signal include level, shape and frequency. These three characteristics will now be discussed in more detail.

Level

Since analogue signals can take on any value, the level gives vital information about the measured analogue signal. The intensity of a light source, the temperature in a room, and the pressure inside a chamber are all examples that demonstrate the importance of the level of a signal. When measuring the level of a signal, the signal generally does not change quickly with respect to time. The accuracy of the measurement, however, is very important. A DAQ system that yields maximum accuracy should be chosen to aid in analogue level measurements.

Shape

Some signals are named after their specific shape – e.g. sine, square, sawtooth, and triangle waves. The shape of an analogue signal can be as important as the level, because measuring the shape of an analogue signal allows further analysis of the signal, including peak values and slope. Signals where shape is of interest generally change rapidly with respect to time, but system accuracy is still important. The analysis of heartbeats, video signals, sounds, vibrations, and circuit responses are some applications involving shape measurements.

Frequency

All analogue signals can be categorised according to their frequency. Unlike the level or shape of the signal, frequency normally cannot be directly measured with a typical data acquisition system. The signal must be analysed using software to determine the frequency information. This analysis is usually done using an algorithm known as the Fourier Transform.

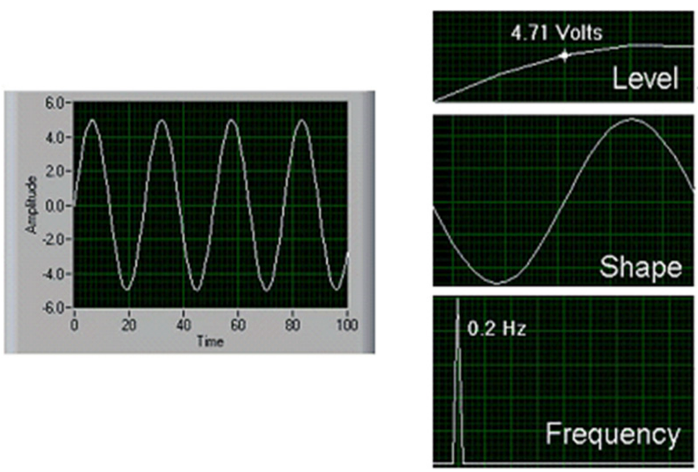


Figure 7.5: An analogue signal with its important characteristics

5.4 Digital signals

A digital signal cannot take on any value with respect to time. Instead, an extended digital signal normally consists of a number of digits (referred to as bits), each of which can take on either of two possible levels: high and low – in the same way that a decimal digit can have one of ten values. Thus, multiple bit digital signals can represent any of a finite number of values, which is a function of the number of bits.

Digital signals generally conform to certain specifications that define characteristics of the measured signal. The useful information that can be measured from a digital signal includes the state and the rate.

State

The shortest digital signal comprises only one digit, having only one of two possible values – referred to as the state of the bit. The state of a digital signal is essentially the level of the signal – on or off; high or low. Monitoring the state of a switch – open or closed – is a common application showing the importance of knowing the state of a digital signal.

Rate

The rate of a digital signal defines how the digital signal changes state with respect to time. An example of measuring the rate of a digital signal is the determination of how fast a motor shaft spins. Unlike frequency, the rate of a digital signal measures how often a signal assumes a specific value.

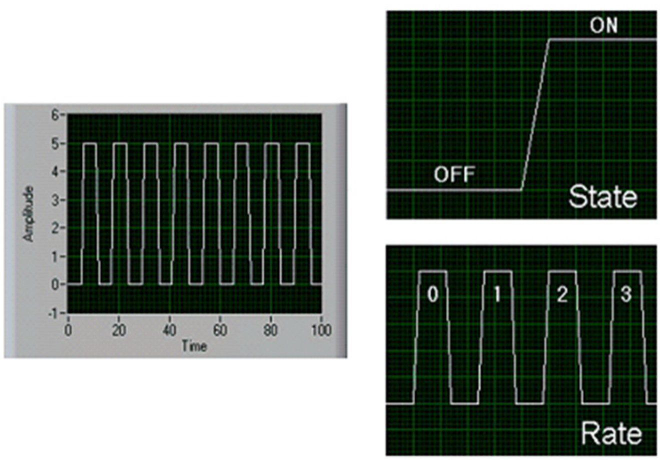


Figure 7.6: A digital signal with its important characteristics

5.5 Signal conditioning

Sometimes, transducers generate signals too difficult or too dangerous to measure directly with a DAQ device; for instance, when dealing with high voltages, noisy environments or extreme high and low (small) signals. Thus, concurrent with signal measurement, signal conditioning is essential for an effective DAQ system. Signal conditioning maximises the accuracy of a system, allows sensors to operate properly, and guarantees the safety of the operator and measuring system.

It is important to select the right hardware for signal conditioning. Signal conditioning is offered in both modular and integrated forms. Signal conditioning accessories can be used in a variety of applications including amplification, attenuation, isolation, simultaneous sampling, sensor excitation, and multiplexing, to name but a few.

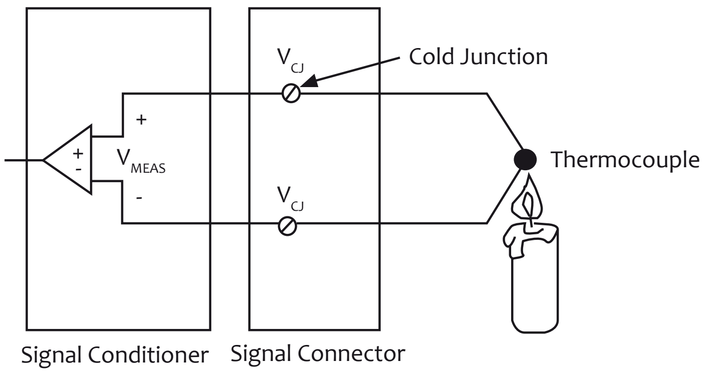


Figure 7.7: A practical signal conditioning setup

5.6 Data acquisition hardware

The DAQ hardware acts as the interface between the computer and the outside world. It primarily functions as a device that digitises incoming analogue signals so that the computer can interpret them. Other data acquisition functionality includes:

- analogue input/output
- digital input/output
- counter/timers
- multifunction – a combination of analogue, digital, counter and timing operations on a single device

The DAQ hardware can be part of different configurations. The most popular configurations are:

- *Distributed*: In this configuration, the sensor and/or actuators are a distance from the PC. The signals are fed via a bus system from the distributed input/output module to the PC.
- *Desktop*: The DAQ hardware (card) is in the desktop computer and signals are fed from the sensor/actuators to the PC via the DAQ card.
- *Portable*: Nowadays, equipment like notebook computers and personal digital assistants (PDA) are used to capture the data – especially when capturing must be done in the field or in an industrial environment far from available DAQ infrastructure.

5.7 Driver and application software

Software transforms the PC and the DAQ hardware into a complete data acquisition, analysis and presentation tool. Without software to control or drive the hardware, the DAQ device will not work properly. Driver software is the layer of software that allows easy communication with the hardware. It forms the middle layer between the application software and the hardware. Driver software also prevents a programmer from having to do register-level programming or complicated commands in order to access the hardware functions.

Data can be acquired and then saved in various different formats. A few of the most commonly used formats are:

- Text
- Spreadsheet
- Excel
- Matlab
- BMP
- JPEG

6. EXAMPLES OF DATA ACQUISITION SYSTEMS

The following are a few examples of DAQ systems that are used to capture data for research projects.

6.1 A flexible control and analysis tool for automatic blood pressure measurement

***The challenge**: to develop a flexible system that performs experiments and blood pressure measurement analysis using the oscillometric method for research and didactical purposes.*

- Creation of the mechanical unit of the device by assembling an occlusive cuff, two pressure sensors, an air pump and an on/off pneumatic valve to control the law of deflation.

- A finger pletismograph and photopletismograph were added to the experimental setup for redundant systolic pressure and arterial pulse wave velocity measurement.
- Development of an application-specific, microcontroller-controlled electronic measurement and display system.

6.2 Structural condition-monitoring system for cable-stayed bridge

The challenge*: to develop a system to acquire and log data from critical areas of a 1.8 km long cable-stayed bridge.*

- Development of a system to measure the output of 100 vibrating wire strain gauges laid on the concrete along the length of the bridge.
- Development of a system to access the vibration of the cable stays in three dimensions using accelerometers.
- Development of an automated, electronic measuring and storing device to acquire and store the measured parameters.

6.3 Racing car performance measurements on a race track

The challenge*: the integration of measured data from various sources in a racing car. The results are to be used in the simulation of particular models of vehicles and tracks to predict performance.*

- Identification of suitable transducers and the placement thereof on all critical positions of the racing car engine and chassis.
- The provision of a suitable radio transmission system for communication with the DAQ system next to the race track.
- The development of a purpose-specific display and recording system as a man-machine interface.

6.4 Measuring the electrical signals of beating heart cells in a culture

The challenge*: measuring the electrical signals from a grid of electrodes in contact with a single layer of beating heart cells in a culture.*

Electrophysiology researchers at Westmead Hospital in Sydney required a system to acquire and analyse signals measured using a microelectrode array. During this study, researchers grew a single layer of heart cells in a culture on an electrode array. As the living cells beat, the researchers obtained valuable information related to heart rhythm disorders from the electrical signals measured in the cell culture. The basic hardware requirements for the system included:

- simultaneous sampling of 64 channels at data rates of up to 70 kHz;
- data storage to a hard disk at the same time as display; and
- high quality graphics for data visualisation.

As biomedical researchers strive to obtain groundbreaking results, they require new analysis tools. In this application, LabVIEW saved considerable software development time in the creation of a new measurement and assessment tool. The hardware provided a platform for researchers to expand upon in the future, thus making the best use of sought-after research funding.

6.5 Testing vehicle temperatures

***The challenge**: a motor manufacturing company needed a compact, portable system to test vehicle temperatures to assure that they do not exceed design limitations in extreme conditions.*

The In Vehicle Data Acquisition System (IVDAS) thermal monitoring system was developed to address the data logging needs of the motor manufacturer. The power of the modern PC coupled with the power of open architecture instrumentation buses opened the door for a powerful and flexible solution. A driver panel allows the test driver to start data logging and alarm processing with the touch of a button.

The software is first set up by defining the channels. This is accomplished in one of three ways:

- A user interface panel allows the user to define channel count, names, scaling, conditioning and alarming.
- A text file can be created and imported with a separate software package, such as MS Excel.
- A company-specific file type can be read into the system to generate a channel list.

Specific setup files can be saved to disk in order to recall them for similar tests at a later stage. After setup, the user can test run the software to look for open or short-circuited sensor circuits. Once setup and initial checkout are complete, the system is ready to be used by the driver. The driver panel allows the test driver to start the data logging and alarm processing with the touch of a button. For safety reasons, no mouse interaction is necessary for the driver. While the driver can pause data acquisition during the test, alarm processing will always be running.

6.6 Displacement measurement

***The challenge**: to measure the displacement of a motorcar tyre when the wheel hits a pothole in the road.*[1]

The measurement was done on the front wheel of a light delivery vehicle.

1 This measurement has been made with respect to the case study described in Chapter 8.

Experimental DAQ System

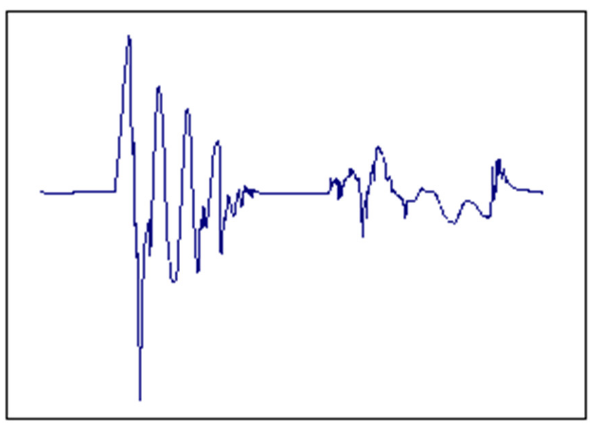
- *Sensor*: The needle of a stereo record player was used to capture the displacement of the tyre during simulated action of hitting a pothole in the road.
- *Signal conditioning*: A pre-amplifier was constructed to amplify the signal from the needle. This was required because the signal from the needle was too small to be captured by the DAQ system.
- *Data acquisition hardware*: A standard data acquisition card from National Instruments was used to capture the data signal from the pre-amplifier.
- *Application software*: LabVIEW data acquisition software from National Instruments was used for the processing and display of the measured parameters.

Since the same manufacturer, National Instruments, provided both the hardware and software, the interfacing between these elements was not a problem. This also had the added advantage that the hardware could be utilised to its full potential and all software features to enhance the data capturing and analysis could be used.

6.7 Using captured data

Normally the captured data can be used with different types of application software to analyse it and to be able to present it in graphical, tabular, or the most suitable form for the researcher. It is for the researcher to decide in what form it will be best suited for analysis and representation. Two different forms of data are shown below in Figure 7.8.

0.000112
0.000499
0.001719
0.002177
0.001872
0.001719
0.002482
0.003398
0.002788
0.002482
0.002177
0.003245
0.002025
0.001262
0.001719
0.002635
0.001719
0.000499



(a) (b)

Figure 7.8: (a) Raw data and (b) Data represented in a graph

A question arises as to what to do if one or two measurements are completely out according to the rest of the data that were captured. The first option will be to repeat the capturing process ensuring that no faults exist within the DAQ System. If the problem still remains, a decision must be made either to ignore that specific data word or to try to determine and explain the possible reasons for the inconsistent data.

7. NEW DATA ACQUISITION TECHNOLOGIES AND ABILITIES

Data acquisition technology provides the link between the data-generating sensors and data-recording and storing devices. DAQ can also provide the means for driving external actuators from a computer by the generation of external excitation signals. DAQ technology includes both hardware and software.

Thanks to recent advancements in processor technology, the low cost personal computer is now the most important carrier for data acquisition cards. The high clock speeds of modern central processing units (CPUs), such as Pentium and PowerPC, enable very high sampling rates. This, along with high performance bus architectures such as PCI, cheap RAM and fast, voluminous hard disks, make long-term continuous measurements possible.

Traditionally, the clock speed of the computer CPU can significantly affect the performance of a DAQ system. However, newer *direct memory access* (DMA) transfer technology speeds up the system by using dedicated hardware to transfer data directly into system memory. Thus, the CPU is not burdened with moving data and is therefore free to engage in more complex processing tasks. In addition, if an application requires real-time processing of high-frequency signals, a dedicated *digital signal processing* (DSP) chip can be built in on the DAQ board to share the workload of the main processor.

Another important development is portable data acquisition based on laptop computers with PCMCIA cards. This configuration allows more convenient field measurements that used to be troublesome for practicing engineers.

Emerging broadband Internet and broadband cellular phones outperform traditional modem hook-ups using RS-232 or RS-485 serial communication ports. These emerging communication technologies will make remote monitoring and access measurements more achievable.

In short, the current level of data acquisition technology, although still not perfect, is far more effective and efficient than it was a decade ago. In future, one can expect even more affordable and accurate measurement instruments, some that could be fitted into computers as small as modern hand-held calculators or personal digital assistants.

8. SUMMARY

Data acquisition is an important component of modern research procedures, and researchers need to be *au fait* with the use thereof. This is the way in which huge amounts of data can be acquired over a long or very short period of time, depending on the nature of the project. The data can then be processed and results displayed or interrogated in different ways by the researcher.

There are many different types of high quality data acquisition equipment and associated software available, meeting a wide variety of possible needs of the researcher. However, due to the specialised nature of the selection and implementation of such technology, it is not uncommon to access the services of a specialist for this purpose. Such an individual would typically have a background in electronics and/or computing and should be able to provide invaluable support to the researcher and enable much quicker progress with this phase of research.

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SECTION 2

Examples of the Uses of Modelling

CHAPTER 8

Data Acquisition and Mathematical Modelling

Anna CM Bekker

1. INTRODUCTION

Mathematical modelling is the use of mathematics to describe and predict phenomena and, although an acceptable procedure in (especially) engineering design, usually requires experimental validation of the ability of the model to predict the behaviour of the system under investigation. This involves the setting up of experimental apparatus and the measuring of the functioning of the system under a set of predefined conditions. Proper assessment of the results obtained in this way assists the researcher in evaluating the quality of the mathematical model used, as well as the appropriateness of the experimental set-up and the external excitation of the system.

The process of modelling is a constant oscillation between various levels of abstraction. This can be divided into the following phases:

- Getting a grip on the problem (define key questions);
- Formulating a mathematical model;
- Generating solutions from the mathematical model;
- Validating the model (and if necessary re-formulating the model until it fits with the real world context).

Whenever possible, the next step in the research process is validation of the mathematical model, by assessing the functioning of the system under investigation by a process of data acquisition and processing. Data acquisition is the process of obtaining and recording primary information from physical experiments, and provides the foundation information on which subsequent data analysis and conclusions are based. The data obtained from physical models helps the researcher to understand the problem under investigation, the model it is represented by, and to verify the validity of the mathematical model.

Being able to utilise ordinary differential equations is essential for professionals in many areas of science and technology. Many useful and interesting phenomena in engineering and life sciences that continuously evolve in time can be modelled by ordinary differential equations, or by a variety of different mathematical procedures [1].

The following describes at length the method employed to study the behaviour of an inflatable car tyre when stimulated externally in a particular way, whilst attempting to minimise the mathematical content of the description.

2. MATHEMATICAL MODELS

While considering a strategy to design tyres to minimise the formation of dirt road corrugations, the following model was considered:

When a vehicle is travelling on a dirt road with uneven surfaces, the contact between tyres and road will not be perfect, and at times the drive wheels will bounce. Before contact of the tyres with the road is lost, the tyres will be under tension (assuming that the vehicle is under power). At the *instant of contact loss*, the tension is released and the tread surface begins to oscillate *tangentially* (parallel to the wheel rim) [2]. The elasticity of the tyre will cause the tread surface to be compressed, owing to a tangential force that is acting on the tread surface of the tyre. The elasticity of the tyre then tends to restore the shape of the compressed tyre. This gives rise to a common tangentially oscillating system relating the tread surface of the tyre, which can be compared to an oscillating system, with the tangential force as the restoring force.

A mathematical model that describes the angular motion of the tread surface of the tyre can be described as a second order differential equation with constant coefficients. The solution to this differential equation gives the angular displacement with respect to time of the tread surface of the tyre. To find the tangential displacement of the tyre's tread surface, the angular displacement (in radians) was multiplied by the effective radius (in metres) of the wheel of the tyre.

The development of the mathematical model describing the phenomena under investigation included practical experimentation – as a consequence of which some constants in the relevant differential equation could be ascertained. The determination of these constants were a primary purpose of the investigation, and the description that follows shows how data captured experimentally can be linked to a mathematical model.

Although the purpose of the shock absorber in a motor vehicle is to cause rapid die-off of vibrations, encountered either randomly or periodically from the natural frequency of the suspension system, the tyre and therefore the tread surface will damp the tangential oscillations that are under investigation.

The value of this damping coefficient (λ) can be determined experimentally by measuring the rate of decay of unforced oscillations or unconstrained motion. The logarithmic method, which is the natural log of the ratio of any two successive amplitudes, could be used to determine the damping coefficient of the tyre [3].

A sequence of actions was taken to measure and assess different characteristics of a tyre, having been exposed to an artificial stimulation similar to what can be expected to take place whilst travelling on a dirt road.

2.1 Case study

It was found that the displacement varies sinusoidally with time, as in the case of simple harmonic motion (SHM), with a frequency ω' and its amplitude, A, being modified by the exponential term $e^{-\lambda t}$, a term which decays with time (t) and the damping coefficient (λ) of the rubber tyre.

Figure 8.1 shows the behaviour of the displacement θ with time – the oscillations gradually decaying with the envelope of the maximum amplitudes following the dotted curve $e^{-\lambda t}$. The constant, A, is obviously the value to which the amplitude would have risen at the first maximum if no damping were present.

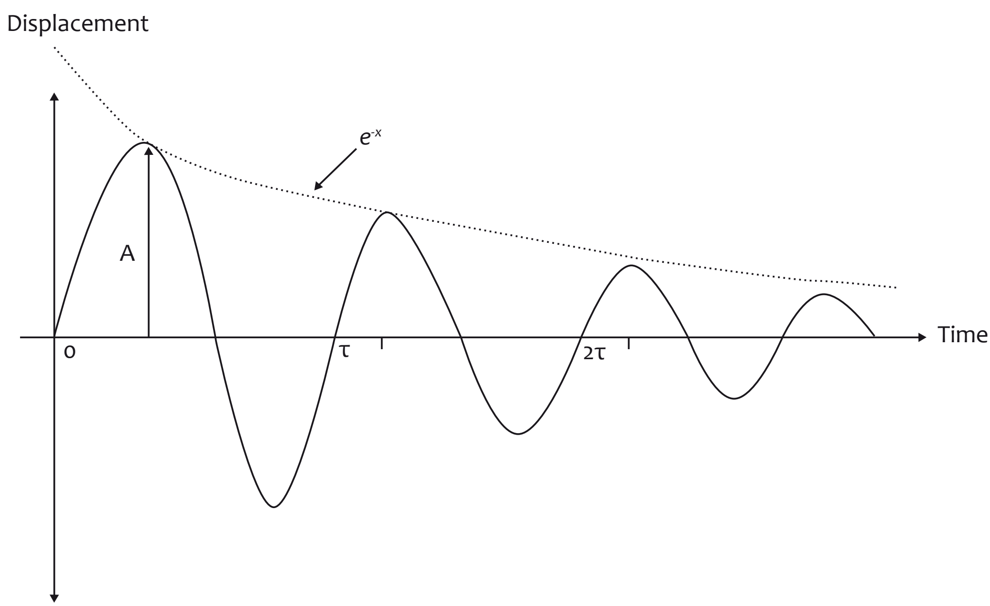

Figure 8.1: Damped oscillatory motion

The presence of a force term in the equation of motion introduces a loss of energy, which causes the amplitude of oscillation to decay logarithmically.

3. LOGARITHMIC DECREMENT

Logarithmic decrement (δ) measures the rate at which the amplitude dies away. Suppose in the expression:

$$\theta = A e^{-\lambda t} \, Sin\left(\omega' t + \phi\right)$$

we choose

$$\phi = \frac{\pi}{2}$$

then

$$\theta = A_0 e^{-\lambda t} \, Cos \, \omega' t$$

With $\theta = A_0 \; ; t = 0$, the behaviour of the displacement will follow the curve, as depicted in Figure 8.2.

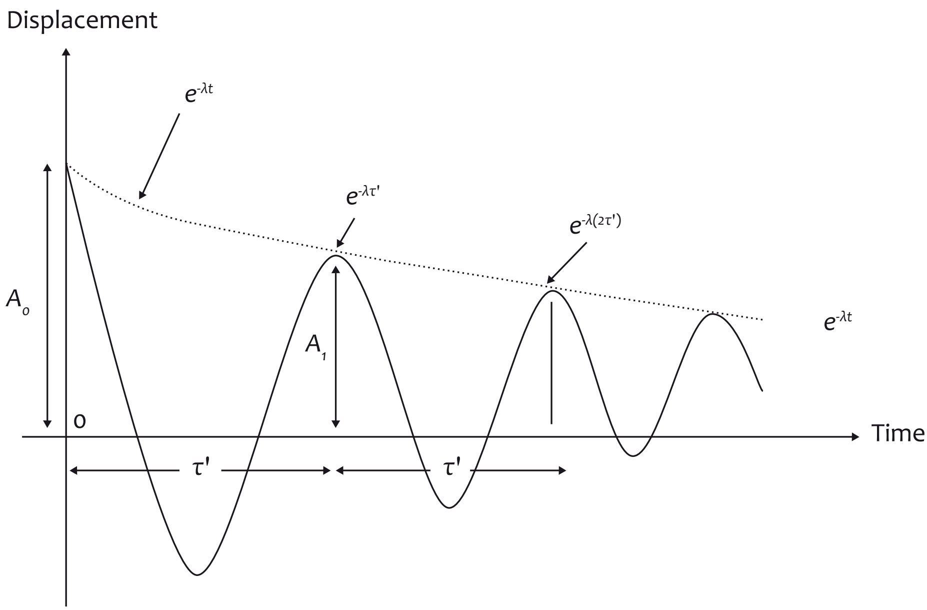

Figure 8.2: The logarithmic ratio of any two amplitudes one period apart is the logarithmic decrement $[\delta = \ln\left(\frac{A_n}{A_{n+1}}\right) = \lambda\tau']$

If the period of oscillation is τ' where $\omega' = \frac{2\pi}{\tau'}$, then the ratio between two adjacent amplitudes can be calculated any number of periods later. Therefore, it is anticipated that a waveform of a similar shape to that in Figure 8.2 will be measured, if a tyre is stimulated in the way described.

3.1 Obtaining data from an experimental physical setup

To find a value for the damping coefficient (λ) of the vehicle's rubber tyre in units of s^{-1}, the following practical experiment was conducted. The experimental method used a typical vinyl record player stylus, a signal conditioning circuit, a data acquisition system and a vehicle. The experiment was done on the front wheel of an Opel Corsa 170i diesel truck.

The vehicle was jacked up to suspend the tyre freely in the air. A typical record player stereo stylus was fastened to a rigid bracket fixed in position so that the stylus touched the tyre's tread surface. The stylus was attached in such a way that its motion was restricted to the horizontal level only. A tangential strike was subsequently delivered to the tyre (approximating an impulse), and the output of the record player stylus via the pre-amplifying circuit captured on a computer with a data acquisition card [4] (see explanatory Figure 8.3 and Figure 8.4).

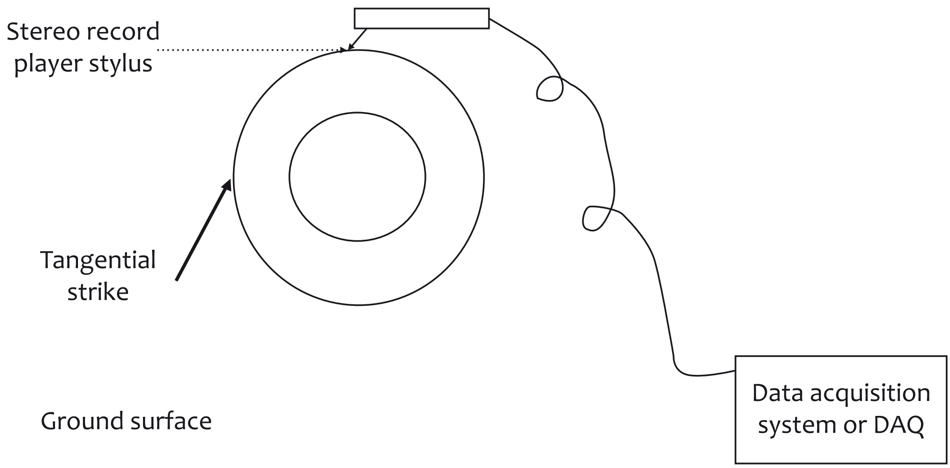

Figure 8.3: Setup of physical experiment

The stylus is shown in Figure 8.4, in a position touching the tread surface of the rubber tyre.

The data that was captured experimentally was imported into Excel to facilitate easy processing and graphical representation. The following graph represents the two channels of the stereo record player stylus as measured:

Figure 8.4: Record player stylus fastened to a rigid bracket, touching the tread surface of the tyre

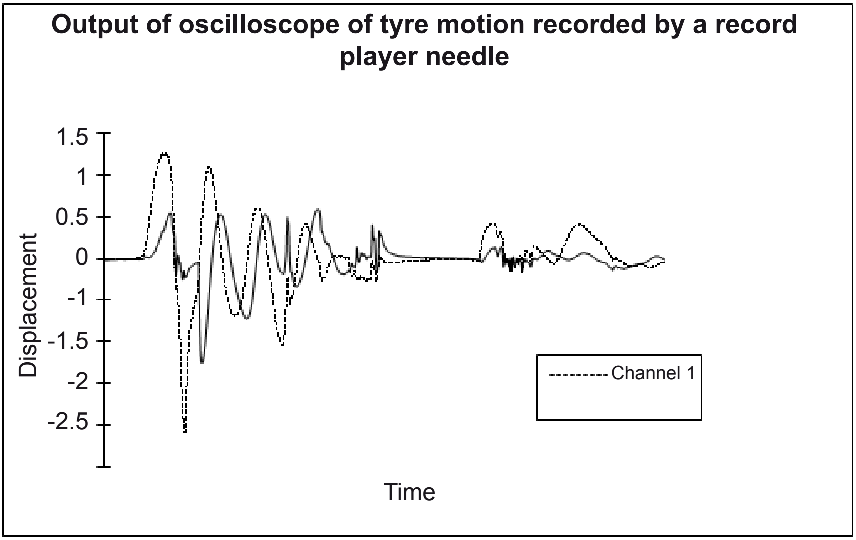

Figure 8.5: Signals captured from a stereo stylus with DAQ when a freely moving tyre was struck by a tangential strike

A stereo stylus was used in order to capture the oscillations of the tread surface of the rubber tyre. This means that the horizontal oscillation of the rubber tyre was captured in two directions, indicated as channel 1 and 2 in Figures 8.5 and 8.6, each forming a 45-degree angle with respect to the horizontal.

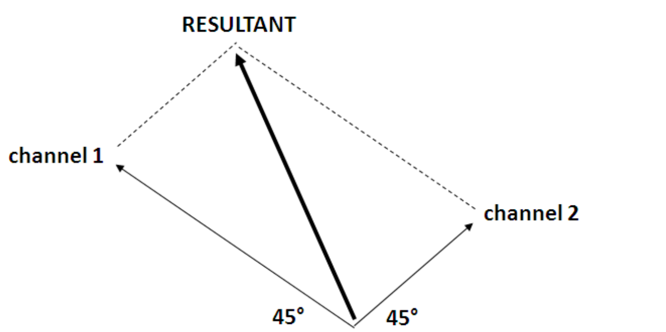

Figure 8.6: Resultant motion of the tread surface of the tyre

The resultant motion is the vector sum of the two channels. Figure 8.6 illustrates the resultant motion of only one sample captured in the experiment (approximately 70 000 samples were taken).

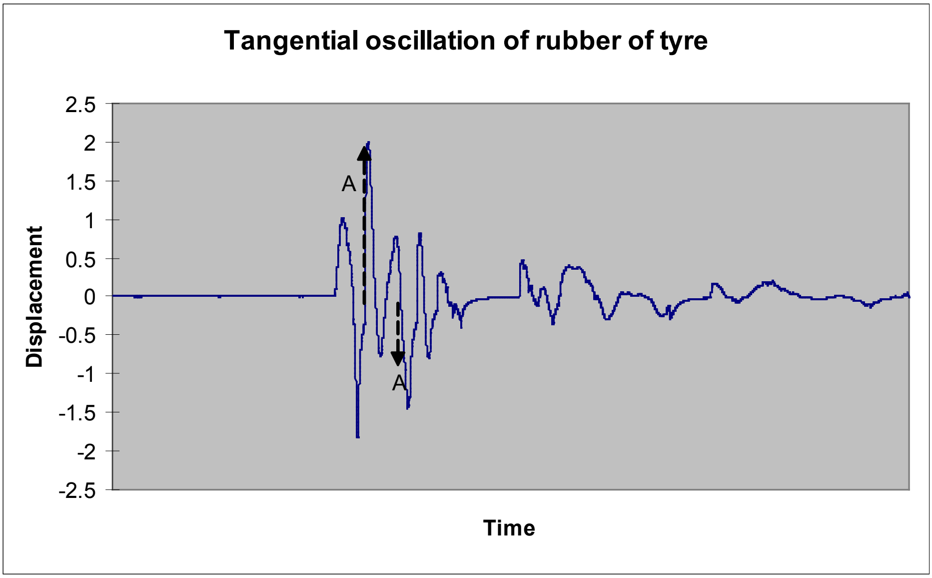

Figure 8.7: Tangential oscillation of the rubber of the tyre when struck by a tangential strike

If this resultant motion is projected onto the horizontal, the horizontal component represents the tangential oscillation of the rubber of the tyre. The horizontal component was now calculated for each sample (MathCad was used for this purpose). Figure 8.7 represents the tangential oscillation of the rubber tyre when struck by a tangential strike.

4. RESULTS

The first maximum amplitude of the impulse is A_o = 1.913 units. The frequency at which samples were taken was every 50 μs = $(50)(10^{-6})$ seconds.

Because 202 samples were taken every 50 μs, the fundamental period of oscillation was $p = (202)(50)(10^{-6})$

$= 0.0101s$

The second maximum amplitude is A_1 = 0.742 units.

The exponential rate of decay δ and hence a value for the damping coefficient (λ) can now be calculated as follows:

Calculation:

$$\frac{A_0}{A_1} = e^{\lambda \tau'}$$

$$\ln\left[\frac{A_0}{A_1}\right] = \lambda \tau' = \delta$$

$$\lambda = \frac{1}{\tau'} \ln\left[\frac{A_0}{A_1}\right]$$

$$= \frac{1}{0.0101} \ln\left[\frac{1.913}{0.742}\right]$$

$$= 187.5\ s^{-1}.$$

Therefore the damping coefficient was found to be: $\lambda = 1.88 \times 10^2\ s^{-1}$.

Thus, it was possible to experimentally verify the validity of the mathematical model of the system, as well as to subsequently calculate the value of important characters thereof.

5. SUMMARY

The following observations were made in determining the damping coefficient of the rubber of the tread surface of the tyre:

- A vibration was induced by a small tangential stroke.
- The vibration energy was dissipated by the material (rubber of the tyre).
- This induced vibration was expressed as a damped sine curve.
- The induced vibration has a frequency spectrum, according to its resonant frequencies, which is dependent on the:
  - elastic properties of the material,
  - geometry,
  - density, and
  - micro and macroscopic structure of the material.
- Each frequency will damp according to the energy absorption of the material.
- The specific damping coefficient is dependent on the dimensions of the specimen.

6. CONCLUSION

The above represents a description of the research procedure used to verify a mathematical model with certain physical characteristics of a system (a rubber tyre in the case under investigation) under specified conditions. The accuracy and validity of the mathematical model was validated experimentally by a process of data acquisition and evaluation, using electronic measuring and recording apparatus.

This study shows that a mathematical model can be a powerful tool in understanding and assessing the operation of complex systems. Data obtained from physical models helps one to understand the model and to verify the validity of the mathematical model. This is a representative example of the use of mathematical modelling as a formal research procedure.

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CHAPTER 9

Numerical Modelling of the Performance of an Industrial Freezer

Tiyamike Ngonda

1. INTRODUCTION

Frost formation is a serious problem in refrigeration equipment such as commercial and industrial freezers. Flat and corrugated-finned tube cooling coils are commonly used in such equipment. If the coil surface temperature is below both the dew point and the freezing point of moist air in the vicinity, frost will form on the coils. Frost growth on the surfaces of cooling coils degrades their performance by blocking the air flow and insulating the surfaces. The state of the air in the vicinity of the coil surface influences both the rate and the nature of the frost that forms. Thus, temperature and humidity ratio are major determinants of frost growth. Many researchers have investigated the effects of these factors on various heat exchanger configurations.

Researchers experimentally investigated the effects of configuration on the performance of flat-finned tube heat exchangers under frosting conditions [1, 9], whilst tests of coils of varying fin pitch and number of rows under subsaturated conditions, with the relative humidity ranging from 40% to 90%, was described in [1]. In this investigation, the air flow was maintained at a constant rate. The results indicate that air flow rate affects frost formation and that the effect of fin pitch is not significant after a certain pitch. Most of the experimental research gives only qualitative indications of the critical factors in heat exchanger performance.

Recently, researchers have focused on the development of semi-empirical and numerical models to predict heat exchanger performance. The models can be divided into steady-state and transient models. Some researchers, such as Seker *et al.* [5] and Xia *et al.* [8], have focused on steady or quasi-steady-state models based on modifications to the standard equations for computing heat exchanger duty. Others have focused on transient modelling of heat exchanger performance. They divided transient models into black-box, one-zone, two-zone and distributed models, whilst some have focused on distributed models and lumped-property models of the performance of heat exchangers under frosting conditions.

In commercial and industrial freezers, coil processes and the inflow of warm outside air result in the development of supersaturated air, a mixture of saturated air and suspended ice crystals or water droplets. Limited work has been done on frost growth under supersaturated conditions, except for the models of Mago and Sherif [2] and Ngonda and Sheer [4] on frost formation on flat plates. None of the previous researchers have modelled frost growth on a complete heat exchanger under supersaturated conditions.

2. MODELLING THE PERFORMANCE OF AN INDUSTRIAL REFRIGERATOR

The physical system of an industrial refrigerator is complex. It comprises sub-systems that provide various functions: mechanical sub-systems that provide the refrigeration, and electrical and control sub-systems that regulate the functioning of components such as the compressors and valves. Analysis of the entire refrigeration system would be both complicated and/or even undesired. Hence, the analysis was limited to a manageable, representative size. This technique of system simplification is a standard procedure in modelling.

2.1 Definition of the domain of interest

In a refrigerator, frost first forms on the coldest surfaces which in most cases are the cooling coil surfaces. The cooling coil surfaces form part of the heat transfer path. The frost results in an increase in the resistance to heat flow and the added resistance reduces the refrigerator performance. Thus, the spatial domain for the model can be reduced to the cooling coil.

As frost builds up on the coil surface, the frost surface temperature increases with an increase in frost thickness, until the surface temperature reaches the freezing point of water. When the surface temperature exceeds the freezing point of water, the surface frost melts and seeps into the frost layer. As it seeps down, it freezes within the frost layer, causing densification of the frost layer. The melting and refreezing of ice is a complex physical phenomenon that still has not been fully modelled. Consequently, the time domain is limited by the frost surface temperature, and the model terminates when the frost surface temperature reaches the freezing point of water.

Like most physical phenomena, modelling the effects of frost growth in industrial refrigerators is a transient, three-dimensional problem. The spatial domain is limited to the cooling coil whereas the time domain is restricted by the frost surface temperature.

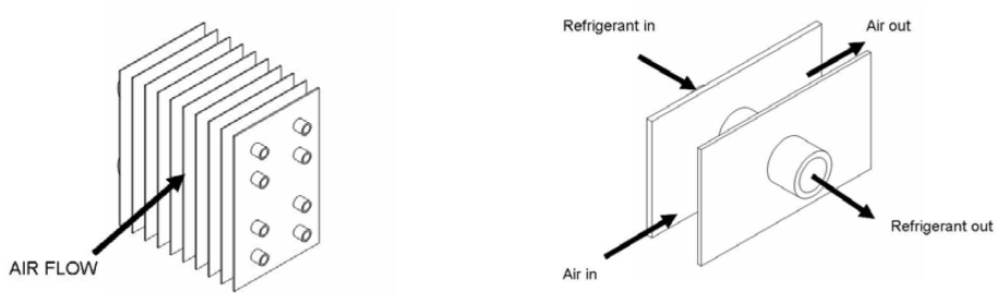
2.2 Development of governing equations

Having established that the cooling coil is the domain of interest, the thermal behaviour of the refrigerator can be modelled by applying the conservation laws to the coil to develop a numerical model. The model is made up of two sub-models, the frost formation model and the heat exchanger model. Although the heat and mass transfer mechanisms are multidimensional and multifaceted, the complex mechanisms can be simplified using the following assumptions:

- The refrigerant is a single-phase liquid.
- A section of the flat-finned tube can be replaced by a pipe with radial fins of rectangular profile based on the procedure laid out in [3].
- Although frost properties vary with frost depth, they can be replaced with layer averaged quantities.
- The thermal resistance of the heat exchanger pipes is very low.

The cooling coil model

The cooling coil can be divided into several control volumes, each comprising refrigerant, tube and fin, and air outside the tube, as shown in Figure 9.1. The governing equations for each of the components of the control volume were then generated.



(a) **(b)**

Figure 9.1: Diagram of a heat exchanger and a single control volume

Energy equation for the refrigerant is given by:

$$\rho_r V_r C_{p,r} \frac{\partial T_r}{\partial x} + \frac{2}{r_p} U_i \left(T_{w,o} - T_r \right) = \rho_r C_{p,r} \frac{\partial T_r}{\partial t} \tag{1}$$

Energy equation for the pipe is given by:

$$C_{p,p} M_p \frac{\partial T_w}{\partial t} = \eta_f A_f A_o h_o \left(T_\infty - T_w \right) + q_f - U_i A_i \left(T_w - T_r \right) \tag{2}$$

The fin efficiency, η_f, is defined by the one-term approximation of Sommers and Jacobi [6]. The approximation accounts for both frost conduction resistance and latent heat effects.

Energy balance for the air side gives equation (3):

$$\frac{\dot{m}_a di_a}{dy} = \frac{h_o A_{o,T}}{C_{p,a}}\left(h_a - h_{fr,s}\right) \tag{3}$$

Mass conservation on the air side gives equation (4):

$$\frac{\dot{m}_a dW_a}{dy} = h_m A_{o,T}\left(W_a - W_{fr,s}\right) \tag{4}$$

The heat transfer coefficient was calculated using a correlation for the Colburn factor, for a flat-finned tube heat exchanger given in [7]. Pressure drop through the coil was calculated using equation (14-48) in [3], whilst the friction factor was evaluated using the equation provided by Wang *et al.* [7] on p.2699. The entrance, *Kc*, and exit, *Ke*, pressure loss coefficients were calculated using correlations based on Figure 14.17 in [7].

The frost model

The frost model can be divided into two main segments:

- The flow on the air side of the frost layer and the heat and mass transfer on the frost-air interface, and
- The process within the frost layer.

On the air side, flow under supersaturated conditions is basically multiphase flow that can be modelled based on principles of particle-laden flow, as outlined in [4]. The air-side model is solved independently of the frost-side model and produces two outputs: the heat transfer coefficient at the frost interface, and the ice accretion rate for supersaturated conditions. The mass transfer coefficient is derived from the heat transfer coefficient, using the heat and mass transfer analogy, as outlined in equation (5). The mass that is transported to the frost interface is then given by equation (6).

$$h_m = \frac{h_o}{\rho C_p Le^{2/2}} \tag{5}$$

$$\dot{m}_t = h_m\left(W_a - W_{fr,s}\right) + \dot{m}_a \tag{6}$$

The frost layer is modelled by coupling the mass conservation equation and the energy equation. As a result of layer averaging, the mass diffusion into the frost layer is given by equation (7). Since the water vapour that is transported to the frost interface either diffuses into the frost layer or deposits on the frost surface, the rate of increase of frost thickness is given by equation (8).

$$X_f \frac{d\overline{\rho}_f}{dt} = \overline{D}_{eff}\overline{\rho}_a \frac{W_{fr,s} - W_w}{X_f} \tag{7}$$

$$\bar{\rho}_f \frac{dX_f}{dt} = \dot{m}_t - \bar{D}_{eff} \bar{\rho}_a \frac{W_{fr,s} - W_w}{X_f} \tag{8}$$

Heat is transported through the frost layer by conduction, and through the water vapour as it diffuses and sublimes into ice within the frost layer, thereby liberating heat. As a result of this internal heat generation, the temperature profile within the frost layer is not uniform. Despite the non-linear temperature profile, the heat that is transported past the cold surface is given by equation (9).

$$q_f = \bar{k}_{fr} \frac{T_{fr,s} - T_w}{X_f} + i_{sub} \bar{D}_{eff} \bar{\rho}_a \frac{W_{fr,s} - W_w}{X_f} \tag{9}$$

Grid layout and discretisation of the governing equations

The nodes are laid out on the inlet and exits for the control volume as shown in Figure 9.2. Equations (1) and (2) are expanded, using Taylor series expansion, to equations (10) and (11) respectively.

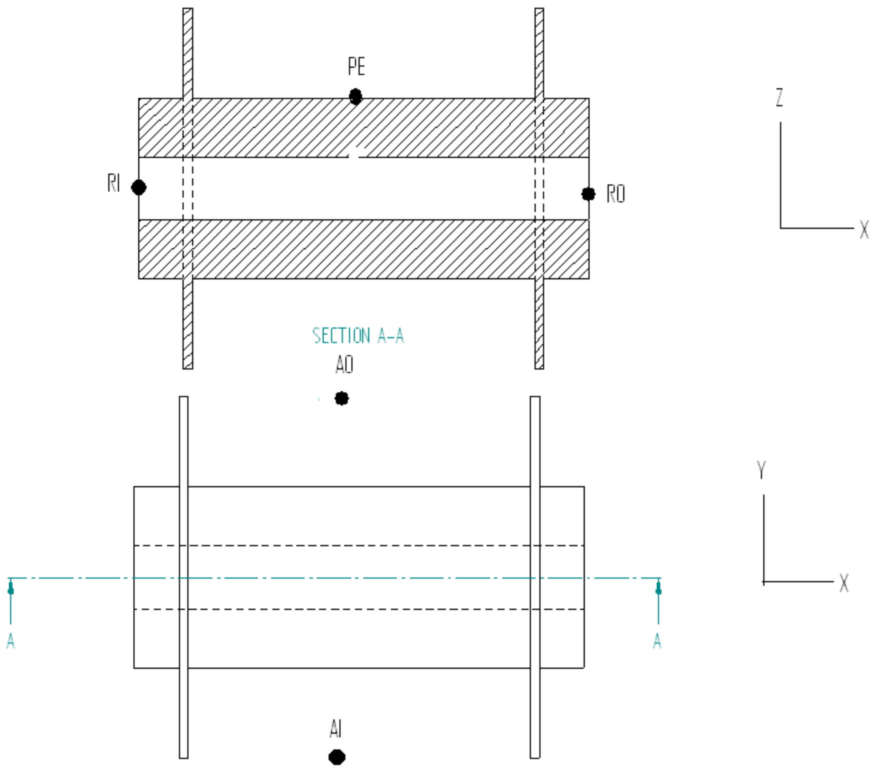


Figure 9.2: Location of nodes in the control volume

$$\rho_r V_r C_{p,r} \frac{T_{r,RO} - T_{r,RI}}{dx} + \frac{2}{r_p} U_i \left(T_{w,PE} - T_r \right) = \rho_r C_{p,r} \frac{T_r^1 - T_r^0}{dt} \tag{10}$$

$$C_{p,p} M_p \frac{T_{w,PE}^1 - T_{w,PE}^0}{dt} = \eta_f A_f A_o h_o \left(T_\infty - {}_{w,PE} \right) + q_f - U_i A_i \left(T_{w,PE} - T_r \right) \tag{11}$$

Development of the algorithm

Solution of the numerical scheme was executed as follows:

- Input initial values
- Calculate property values
- Solve equations 10 and 11
- If $T_w < 0°C$, then solve equations 7, 8 and 9, else go to 6
- Update equations 10 and 11
- If $T_{w1} – T_{wo} > 0.001$, go to 4
- Solve equations 3 and 4
- Use the exit condition for the first control volume as the inlet conditions for the next control volume
- Go to 2.

Development of a computer programme to implement the algorithm on a computer

The algorithm was implemented in Matlab. The algorithm generated a lot of data and, consequently, the main issue in the code development was data storage.

3. RESULTS FROM THE NUMERICAL MODELLING

Figures 9.3 and 9.4 show the variation of coil duty, with time for various super saturation ratios. They all indicate that coil duty decreases with time. As frost builds up on the coil surfaces, two problems arise. Frost blocks the air passages in the coil and, consequently, increases the pressure drop with time. The increase in pressure drop causes the air flow rate to decrease, which in turn results in reduced capacity for the coil. Frost on the coil surface also results in an increased heat flow resistance, thus reduced capacity.

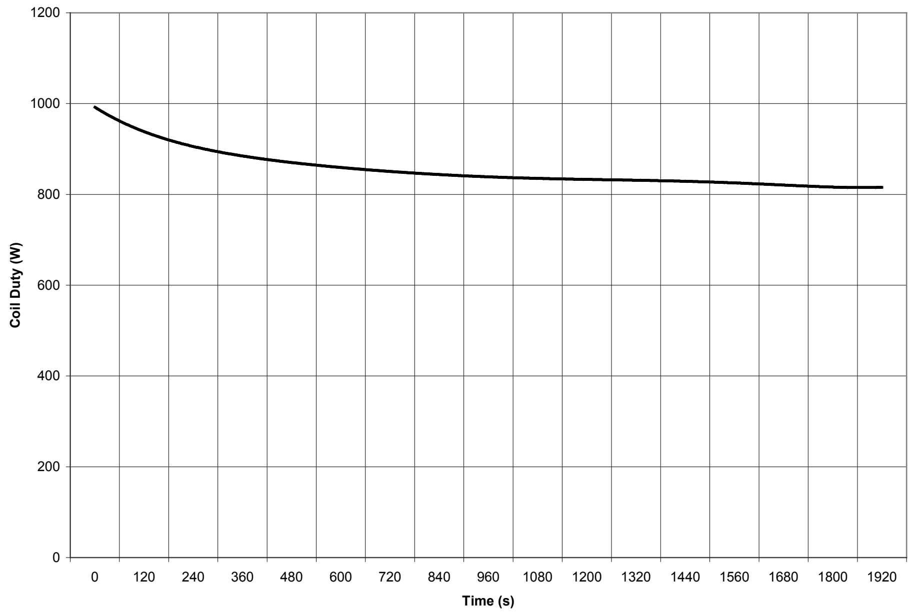


Figure 9.3: Coil duty [W] for supply air at 0°C and S = 32%

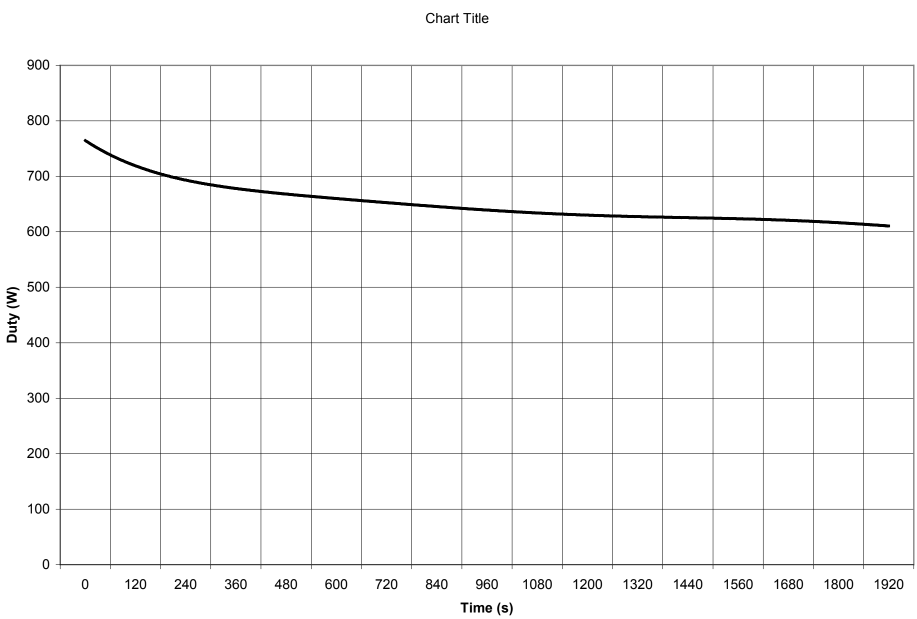


Figure 9.4: Coil duty [W] for supply air at -4°C and S = 8%

Inspection of Figures 9.3 and 9.4 indicates that coil duty reduces by about 15% in 30 minutes, and then evens out slightly. Designers of refrigeration equipment usually oversize cooling coils by as much as 50%. A reduction of 15% is well within this range. As indicated in literature, the frost that initially forms on the coil surfaces is less dense, and can be defrosted in a few minutes. The frost which forms after numerous cycles of melting and refreezing of the frost layer is dense and difficult to defrost. The numerical results seem to indicate that a defrost cycle of 30 minutes or more would be appropriate, as the reduction in coil performance is within the design limits and cycling melting and refreezing has not set in.

More work is, however, required before design guidelines for defrost cycles can be laid out. There seems to be an indication from other literature that short cycles would enable a decrease in the overdesign of cooling coils to less than the current 50%.

The model presented here is based on distributed principles for the heat exchanger model and layer-averaged properties for the frost model, and proposes a short defrost cycle.

4. CONCLUSION

From the above, it is apparent that the operational characteristics of a physical device, such as a sub-system of an industrial refrigerator, could be modelled mathematically, rendering an improved understanding of the functioning of the system.

Using such techniques, it is possible to identify (potential) deficiencies in the design of a particular system, or general design practices of systems of similar characteristics. Likewise, modelling can also be used for the optimisation of designs, as well as the prediction of the expected functioning of new designs.

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6. NOMENCLATURE

C_p	Specific heat capacity (J/kgK)
D	Diffusion coefficient (m/s)
h	Heat transfer coefficient (W/m^{2}K)
I	Enthalpy (J/kg)
m	Mass of pipe (kg/m)
q	Heat flow rate (W)
r	Radius (m)
S	Supersaturation = $(W - W_{sat})/W_{sat}$ (%)
T	Temperature (K)
U	Overall heat transfer coefficient (W/m^{2}K)
V	Velocity (m/s)
W	Humidity ratio (kg_{water}/kg_{air})
Greek:	
ε	Porosity
η_f	Fin efficiency
ρ	Density (kg/m3)
Subscripts:	
a	Air
eff	Effective

f	Fin
fr	Frost
i	Inside
m	Mass
o	Outside
r	Refrigerant
s	Surface
sat	Saturation
sub	Sublimation
T	Total

CHAPTER 10

Coupled Hydrological and Agent-based Modelling for the Understanding of Human-Environment Dynamics

Y.E. Woyessa and W.A. Welderufael

1. INTRODUCTION

The planning and management of water resources at a catchment level is becoming a widely adopted approach [5]. This approach enables monitoring of the water balance of a hydrologically isolated catchment [5]. The delineated surface environment helps to reconcile the input and output of water in the system. In addition, the different biophysical and social interactions and processes that are taking place and that have a significant effect on water resources can be spatially identified [11].

In a given catchment, the natural resource in general and the water resource in particular can be affected by several factors, such as biophysical (precipitation, temperature, ground water flow, vegetation, soil type and topography) and socio-economic factors (institutions, technological developments, markets, etc.). These, in turn, have a combined effect on land use and impact on the water resource. The change in land use takes place as a result of decisions by land users, which in themselves are a consequence of the interactions between the socio-economic and biophysical factors.

Different land types and associated contrasting soils contribute to differences in runoff, surface evaporation, and recharge that take place on a catchment scale. The direct response of a rainfall event which is runoff may route the natural canal system and discharge at the outlet of a catchment, or be harnessed by a reservoir for different uses.

Individual land owners operating in a catchment undertake complex processes of interaction between the natural environment and the socio-economic situation. The biophysical input largely relates to the climate and soil properties; and these are largely beyond human control. Thus, the final decision to change land use can only be reached after a complex interaction of socio-economic and environmental factors have been considered. For a given catchment, the detailed process of these interactions can be rationally conceptualised in a multidisciplinary way.

The new paradigm in land use decision-making requires greater consideration of the complex human (agents) and environment interactions. In the broader sense, land use and cover change is a result of a human decision that emerges from the interactions of agents, biophysical inputs and the environment [6]. Hence, human decision-making plays a major role in land use change. Land use change can bring about a significant effect on a catchment water resource. For instance, it has been demonstrated, using an empirical model, that a decrease in runoff contribution of 25.3% would occur if all suitable lands for Rain Water Harvesting (RWH) were put under cultivation in C52A (one of the quaternary catchments in the Modder River basin), which would most likely affect the downstream water supply [11].

2. AGENT-BASED MODELLING

Over the past few decades, numerous researchers have improved measurements of land use change using predictive models that can describe significantly more complex processes of land use and their impact on water resources [3, 6]. Understanding the causes of land use change has moved from simplistic representations of a few driving forces to a much more profound understanding that involves situation-specific interactions among a large number of factors at different spatial and temporal scales. These models have modules for the socio-economic as well as for the biophysical inputs [3]. Agent-based models developed for land use/cover change are equipped with two important key components: the cellular model that represents the landscape under study; and an agent-based model (ABM) that represents human decision-making and interactions [1].

According to Berger *et al.* [1], ABM consists of autonomous decision-making entities (agents), an environment through which agents interact, rules that define the relationship between agents and their environment, and rules that determine a sequence of actions in the model. Furthermore, three classes of models that deal with Common Pool Resources (CPR) are identified as [3]:

- physical models centred on the dynamics of resources and that consider demand as a given parameter;
- agronomic, economic or agro-economic models centred on demand and that attempt to adapt water demand to a fixed amount of resource; and
- mixed models that represent interaction between the functioning of physical and socio-economic systems through a single mathematical language.

This is done through the coupling of several models or through multi-agent systems (MAS). ABMs integrate the first two models and are represented by the third type of model.

Several researchers have constructed land use scenarios and estimated discharge from a catchment by using hydrological or agro-economic models [7, 9]. In an ABM perspective, different scenarios of land use and land use change decisions are made by the agents (farm managers) in the virtual laboratory of the ABM model that mimics the actual situation through the rules and communication system conceptualised by multidisciplinary scientists, based on the real situation of the environment.

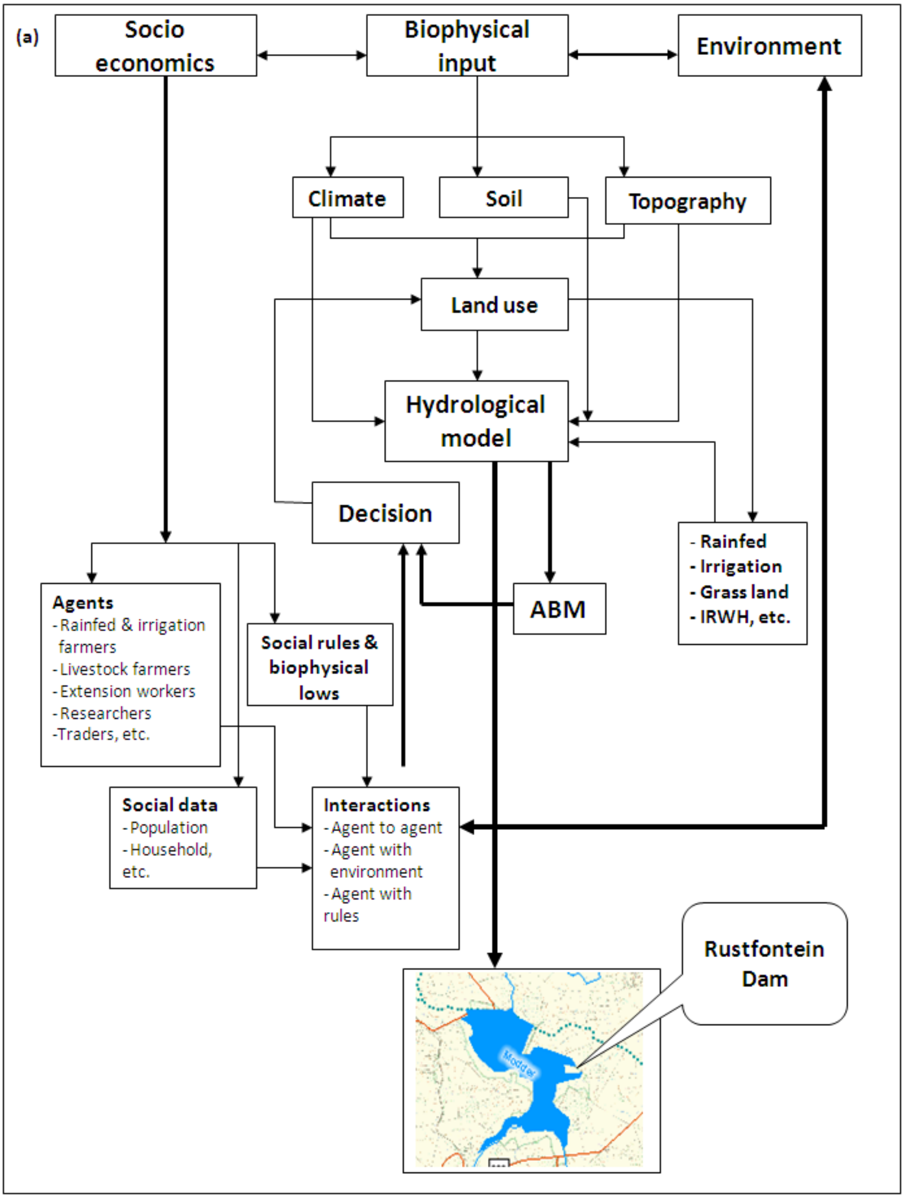

Figure 10.1: Conceptual model of land use decision and its impact on water resources: (a) upstream, and (b) downstream of Rustfontein dam [10]

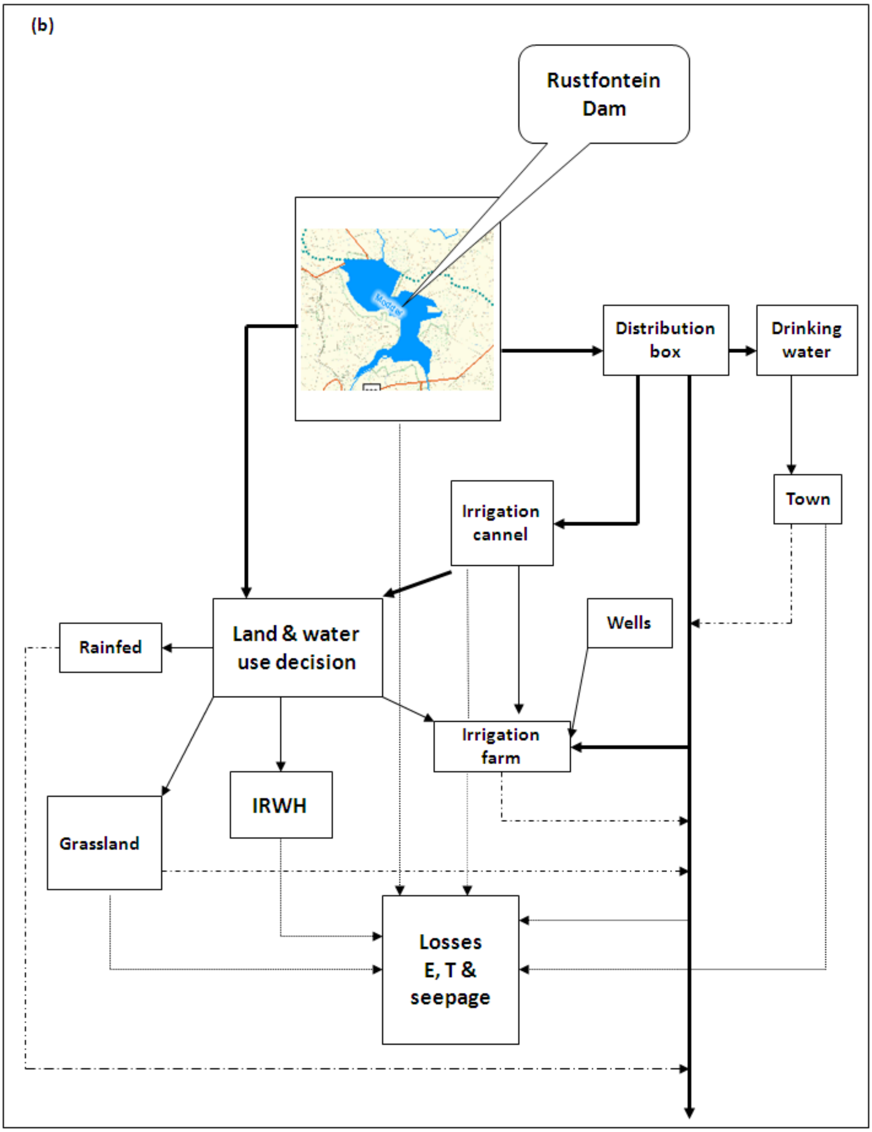

Figure 10.1 (continued): Conceptual model of land use decision and its impact on water resources: (a) upstream, and (b) downstream of Rustfontein dam [10]

3. HYDROLOGICAL MODELLING

The impact of land use changes on ecosystems and biodiversity have received considerable attention from ecologists, and evidently, land use changes in a catchment can impact on water supply by altering hydrological processes such as infiltration, groundwater recharge, base flow and runoff [8].

One of the water supply sources in a river basin is stream flow, which plays an important role in establishing the critical interactions that occur between biophysical, ecological, and socio-economic processes. Socio-economic processes including population dynamics, land use transformation, migration, transportation, and agricultural practices closely interact with and greatly affect ecological processes, such as vegetative growth, ecological succession, and habitat formation and maintenance [2].

Hydrological dynamics can be used as a medium of understanding the conditions for interactions to take place and the consequences that arise from such interactions. One of the most important socio-economic processes for establishing far-reaching and long-term environmental effects is land use transformation, especially the human-induced variety termed 'urbanisation'. The far-reaching effects of urbanisation can best be described by its enormous impacts on basin hydrology and water quality. Understanding these complex socio-hydrological dynamics is imperative for planning a more sustainable future. For instance, covering large watershed areas with impervious surfaces frequently results in increased surface runoff and reduced local surface erosion rates. Moreover, watershed development changes land use patterns and reduces base flow by changing groundwater flow pathways to surface water bodies [8].

Numerous modelling approaches have been developed to simulate the impact and consequences of land use changes on the environment in general, and water resources in particular. One of these models is called the Soil and Water Assessment Tool (SWAT), and is used in the assessment of impact of land use and land-cover changes on water resources.

SWAT is a basin scale model that operates on a continuous daily time step and is designed to predict the impact of management on water, sediment and agricultural chemical yields in ungauged catchments. The model is physically based and capable of continuous simulation over long time periods. Major components of the SWAT model include weather, hydrology, soil properties, plant growth, and land management. In the SWAT model, a catchment is divided into multiple sub-catchments, which are then further subdivided into hydrologic response units (HRUs) that consist of homogeneous land use, management, and soil characteristics. The HRUs represent percentages of the sub-catchment area and are not identified spatially within a SWAT simulation. Alternatively, a catchment can be subdivided into sub-catchments that are characterised by dominant land use, soil type, and management [4].

Example of SWAT application

The SWAT model was applied to the Modder River basin of Central South Africa to evaluate the impact of land use change on water resources, with particular emphasis on the flow of water into Rustfontein Dam. According to the drainage classification of South Africa, the Modder River basin falls within the tertiary catchment called C52. This is further divided into quaternary catchments, such as C52A, C52B, etc. Rustfontein Dam is located in the upper part of the Modder River basin (see Figure 10.2) with a contributing area of 92 761 ha, which is the area of C52A.

As indicated above, the inputs to the SWAT model are land use types (such as agriculture, both irrigated and dry land), forest, rangeland (improved and non-improved, pasture, grass land, shrubs, etc); topography in the form of a Digital Elevation Model (DEM); soil characteristics (such as hydrological soil groups, maximum root zone depth, soil bulk density, soil saturated hydraulic conductivity, and soil available water capacity); and weather data (such as daily rainfall and temperature). Two sets of land use data for the years 1994 and 2000 were obtained from the Institute for Soil, Climate and Water of the Agricultural Research Council. The preparation of input data for the model was one of the most demanding, but important, aspects of the overall task.

Keeping all the parameters, such as soil, topography, and climate, constant, the impact of land use change on water resources was evaluated using the SWAT model. The comparison of land use data for both years and the percentage of change in land use type and/or cover are given in Table 10.1.

Table 10.1: Land use types during the year 1994 and 2000, and percentage of change during this time [1]

Land Use	1994 (Ha)	2000 (Ha)	Difference (Ha)	%
Pasture (PAST)	70 854	78 044	7 190	10
Range-Brush (RNGB)	9 446	4 175	-5 271	-56
Agricultural land row crops	10 261	7 214	-3 047	-30
Evergreen forest (FRSE)	31	223	192	619
Wet land (WETN)	200	1 379	1 179	589
Water (WATR)	1 752	1 048	-704	-40
Urban (URBN)	138	599	461	334
Sum	92 682	92 682		

1 Note: The land use types are prepared and classified according to the input requirement of the SWAT model.

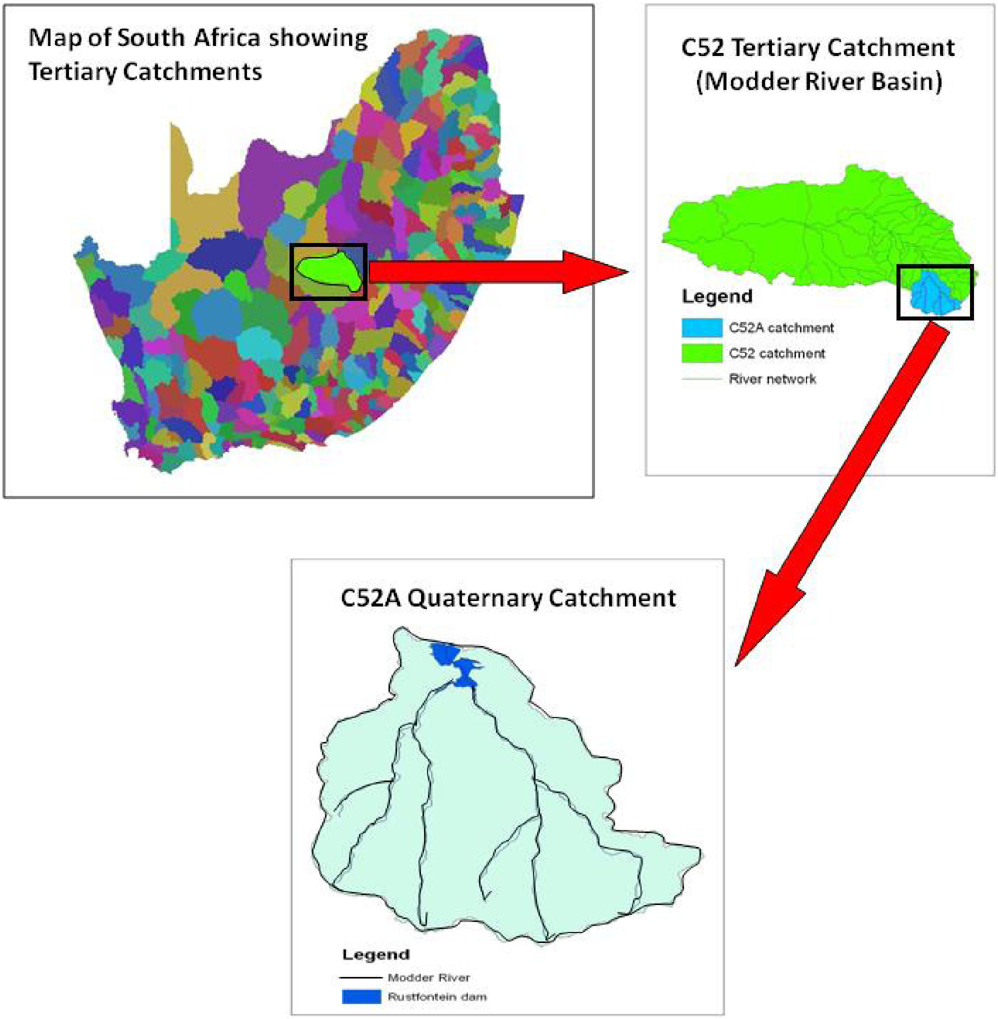

Figure 10.2: Location of the Modder River basin and the study area (C52A)

The model was used to simulate several parameters, among which the surface flow (SURQ), the base flow (GWQ), and the water yield were selected for evaluation purposes. Table 10.2 and Figure 10.3 show the variation of these parameters for the two land use data sets.

Table 10.2: Simulated parameters based on land use data sets of 1994 and 2000

(a) Using land use data of 1994

Year	Precipitation (mm)	Direct surface flow (mm)	Groundwater flow (mm)	Water yield (mm)
1999	433.5	84.89	11.22	95.44
2000	677.0	141.46	122.50	263.06
2001	1021.7	265.80	167.96	432.31
2002	689.0	144.42	141.19	284.80
2003	433.4	99.04	66.94	165.58
2004	541.0	88.31	59.00	146.51
2005	677.7	119.73	105.29	223.70
2006	1218.9	405.30	223.55	627.15
2007	522.3	76.58	48.66	124.51

(b) Using land use data of 2000

Year	Precipitation (mm)	Direct surface flow (mm)	Groundwater flow (mm)	Water yield (mm)
1999	433.5	101.70	11.52	112.43
2000	677.0	169.94	132.75	301.59
2001	1021.7	316.81	182.78	497.84
2002	689.0	173.50	153.39	325.93
2003	433.4	118.28	72.48	190.28
2004	541.0	106.72	63.82	169.61
2005	677.7	145.32	113.15	256.87
2006	1218.9	478.67	244.55	721.18
2007	522.3	93.56	51.57	144.27

The results showed that there was an average increase in water yield by about 15% over a period of nine years (1999-2007), when land use data of 1994 was compared to the land use data of 2000. The increase in water yield was accompanied by a slight increase in settlement areas, an increasing trend in grass land areas (77% to 84%), and a decrease in agricultural areas (11% to 8%).

The difference in water yield given in millimetres per year seems very small. But due to the large area of the catchment (92 761 hectare), a millimetre difference in water yield brings about a volume difference of 927 610 m^3 of water per year, which is a significant amount. The graphical representation of the water yield during these two periods (1994 and 2000) is given in Figure 10.3. The parameter values in general, and water yield in particular, which are given above and in the figure below, are simple simulation values obtained for a model setup and for relative comparative purposes.

The next step in the ongoing modelling exercise is to run the sensitivity analysis in order to identify those parameters that are highly sensitive in affecting the output values. Once the sensitivity analysis is done, then the model needs to be calibrated using observed values, during which sensitive parameter values are obtained for hydrological simulation.

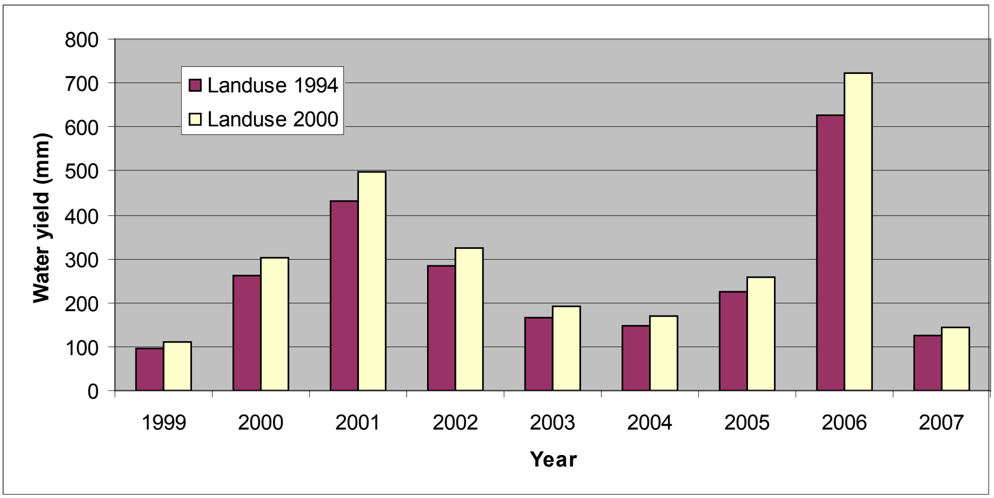

Figure 10.3: Comparison of the simulated annual water yield for the year 1999- 2007 based on the two land use data sets

4. LINKING ABM WITH A HYDROLOGICAL MODEL

In the study of land use changes and their impact on water resources, there are several agents who have a direct and indirect impact on land use decision-making processes. As the number of agents increases, the level of model complexity also increases. However, in order to get the first glimpse of the dynamics of human-environment interaction, the number and type of agents will be limited to farmers, land owners or farm managers, who are directly involved in the use of land in a catchment.

In a given time, a farmer's land use decision is subject to environmental conditions, which in this study are grouped under three categories, namely biophysical, social and economic environments. It is hypothesised that, based on the perception about the environment, individual farmers will take action according to their goals. This action will also be supplemented with interactions and communications with other farmers, in order to arrive at a decision on land use. The outcome of this land use decision will then be linked to a hydrological model to assess the impact of a given land use scenario on water resources. It is planned that the land use scenario results from the ABM will be dynamically incorporated into the hydrological model. The schematic representation of the ABM and its linkage with the hydrological model is shown in Figure 10.4.

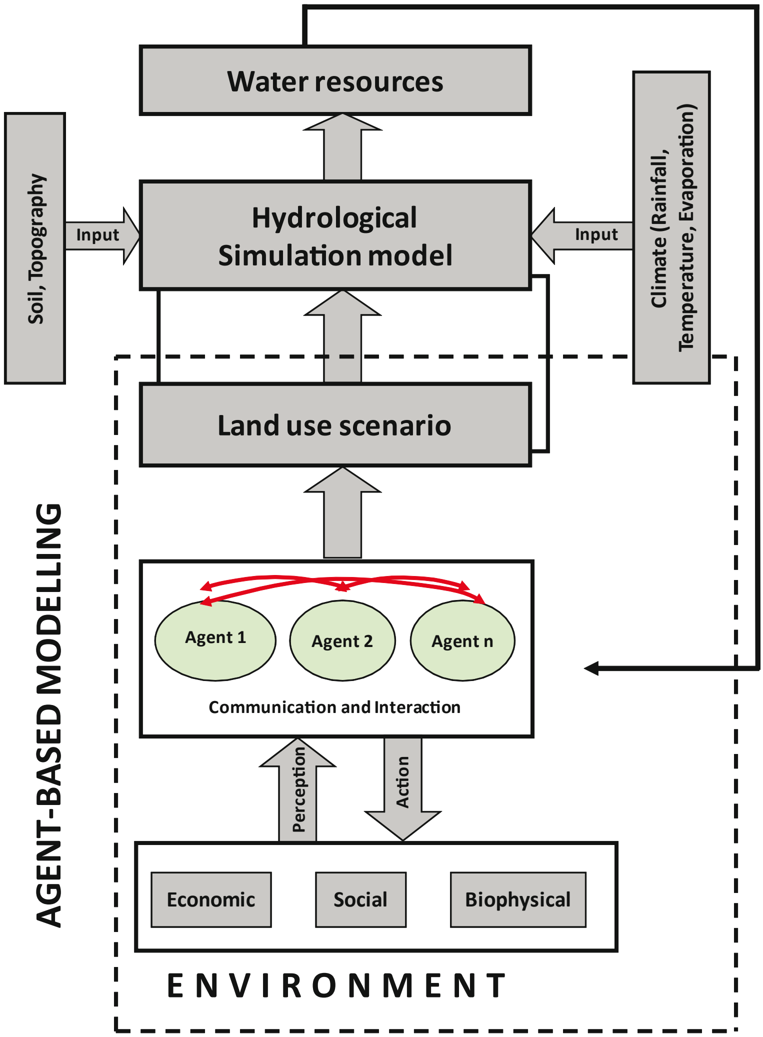

Figure 10.4: ABM and its linkage with the hydrological model

5. CONCLUSION

Individual land owners or managers operating in a catchment interact with the natural environment and the socio-economic situation. The biophysical inputs relating to the climate, soil and topography are largely beyond human control. The final decision to change land use by a land owner can only be reached after a complex interaction of socio-economic and environmental factors have been considered. The detailed process of these interactions can be rationally conceptualised by a multidisciplinary approach. A conceptual model of the consequence of land use decisions on water resources, such as the one presented in this paper, is a step towards an understanding of the dynamics of human-environment interaction.

It is important to note that land use and land cover changes in a catchment impact on water supply by altering hydrological processes such as infiltration, groundwater recharge, base flow, and runoff, which have direct and indirect effects on stream flow in a river basin. Stream flow in a river basin plays an important role in establishing the critical interactions that occur between biophysical, ecological, and socio-economic processes. In such cases, hydrological dynamics can be used as a medium to understand the conditions for interactions to take place and the consequences that arise from such interactions.

Numerous modelling approaches have been developed to simulate such interactions and their impact on water resources. One of the approaches could be the use of a coupled agent-based model with a suitable hydrological model, which can be used to simulate "real world" scenarios of land use change and its impact on water resources on a real time basis. The latter approach is still in a developmental stage and if successful, it could contribute towards a better understanding of the human-environment dynamics and their impact on water resources.

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CHAPTER 11

Neural Network Model Prediction of Short-term Electrical Load Demand

Lucas Nigrini

1. INTRODUCTION

Electric load forecasting is one of the principal functions in power systems operations. The inspiration for accurate forecasting lies in the nature of electricity as a service and trading article, since it cannot be stored. For any electric utility, an estimate of the future demand is necessary to manage the electricity production in an economically reasonable way, so as to meet peak demands without unnecessary load shedding or power cuts [4].

A variety of different statistical load forecasting models have been developed. Practically, there is a subtle difference in conditions and needs of every situation where there is a need for electric load demand forecasting. This has a significant influence on the choice of the appropriate forecasting model.

The majority of the recently reported forecasting approaches are based on neural network techniques, and many researchers have presented good results. The attraction of these methods lies in the assumption that neural networks are able to learn properties of the load which, to discover this otherwise, would require careful analysis by the researcher.

However, research on the neural applications is not complete, and the lack of relative results on different model variations is a problem. To make use of the techniques in a real application (e.g. Bloemfontein City), a comparative analysis of the properties of different neural models seemed necessary.

The system's electric load to be forecast is a random, non-stationary process composed of thousands of individual components. Usually, the only possibility of predicting the future load is to take a macroscopic view on the problem, and try to model the future load as a reflection of earlier behaviour of the system (e.g. "time series prediction"), using an appropriate statistical tool. This still leaves the field open to a number of diverse solutions. Because of the nature of the load, the only objective method to evaluate the approaches is through experimental confirmation.

Extra **S**hort-**T**erm **L**oad **F**orecasting (**ESTLF**) can be used to address this problem. One reason is that recent scientific innovations have brought in new approaches to solve the problem. Recent developments in computer software and technology have broadened the possibilities for solutions, working in a real-time environment. Genetic algorithms, neural networks, expert systems, and fuzzy logic are some of the software tools used to find possible solutions in predicting the electric load "up front" [2].

Objective of study

The objective of the study to be described was to investigate the accuracy of a robust neural tool that can be used to estimate the future electric loads, based on the historical electric load data patterns available from previous statistics.

This study was conducted using historical power load data from the Mangaung area.

2. NEURAL NETWORKS IN LOAD FORECASTING

2.1 Artificial neural network structure

An artificial neural network consists of a number of very simple processors, also called neurons, which are analogous to the biological neurons in the brain. The neurons are connected by weighted links passing signals from one neuron to another.

The output signal is transmitted through the neuron's outgoing connection. The outgoing connection splits into a number of branches that transmit the same signal. The outgoing branches terminate at the incoming connections of other neurons in the network. The neuron inputs may consist of a batch (vector) of binary, continuous, or real numbers [5].

2.2 The perceptron

Now a specific synthetic neuron, the perceptron, is considered, based on the Mcculloch and Pitts model. The perceptron is the simplest form of a neural network and consists of a single neuron with adjustable synaptic weights and an activation function called a hard limiter or threshold function.

The neuron computes the weighted sum of the input signals and compares the result with a threshold value, θ. If the net input is less than the threshold or bias value, the neuron output is -1. But if the net input is greater than or equal to the threshold, the neuron becomes activated and its output value becomes +1. This situation is referred to as the neuron having "fired". This type of activation function is called a sign or threshold function.

The neuron in Figure 11.1 uses the following output or activation function:

$$X = \sum_{i=1}^{n} x_i w_i \qquad Y = \begin{cases} +1, & \text{if } X \geq \theta \\ -1, & \text{if } X < \theta \end{cases}$$

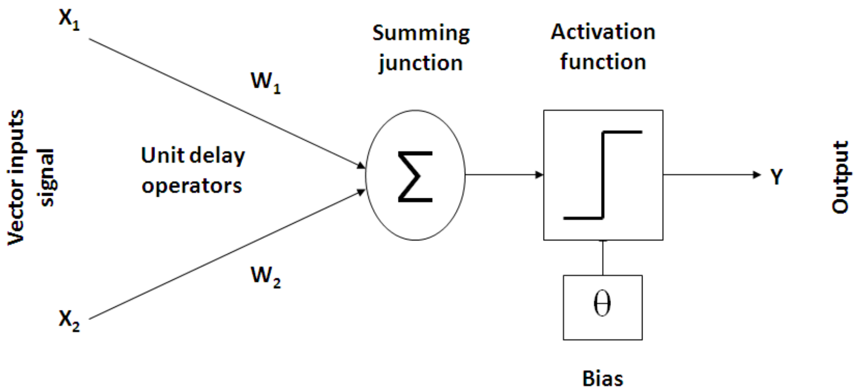


Figure 11.1: Single layer, two input linear threshold perceptron

2.3 Basic activation functions

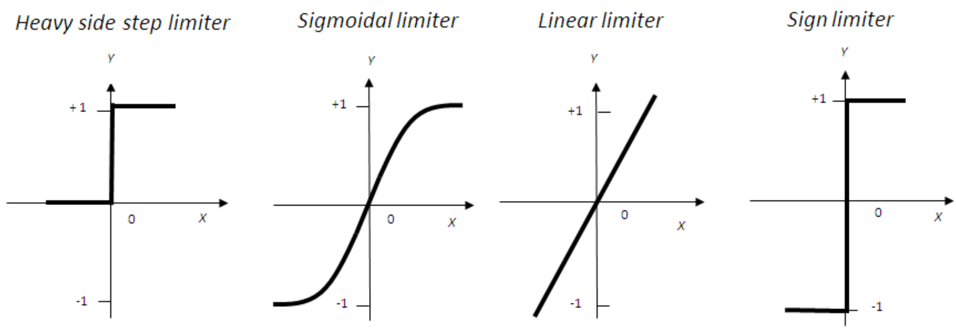
Many different types of linear or non-linear activation functions (or limiters) can be designed [6]. Choosing the correct function depends on the particular problem to be solved. A basic reference model for the presentation of activation functions is shown in Figure 11.2 [5].

Sigmoid functions, shown in Figure 11.2, are the most commonly used functions in the construction of artificial neural networks [7]. They are also known as "squashing functions", thought of as slowly softening the Sign function [8]. This type of function is non-linear and differentiable everywhere, causing greater weight change activity to take place for neurons where the output is less certain (i.e. close to 0.5 where the slope is the steepest) than those in which it is more certain (i.e. close to 0 or 1) [9].

This type of non-linearity is very important, because otherwise the input-output relationship of the network will be reduced to that of a single layer perceptron network [7]. Interestingly, artificial neurons containing sigmoidal functions resemble a type of biological neuron found in the brain [10].

3. NETWORK ARCHITECTURES

A single perceptron is not very useful because of its limited mapping ability. No matter what activation function is used, the perceptron is only able to represent an orientated ridge-like function. Multiple perceptrons can be connected as building blocks of a larger, much more practical, structure called an artificial neural network. Neural networks are complex, non-linear mapping tools. The exciting feature is that a neural net can deal with complex non-linearities in a fairly general way [10, p. 2].



$$f(x) = \begin{cases} 1, \text{ if } x \geq 0 \\ 0, \text{ if } x < 0 \end{cases} \qquad f(x) = \frac{1}{1+e^{-x}} \qquad f(x) = x \qquad f(x) = \begin{cases} +1, \text{ if } x \geq 0 \\ -1, \text{ if } x < 0 \end{cases}$$

Figure 11.2: Four basic types of activation functions

Many kinds of neural networks exist today, and variations of older structures are invented regularly [11].

Neural network structures range widely in type. The selection or design of a particular network depends on the characteristics of the intended application. One of the well-known connection structures is discussed below [7].

4. MULTILAYER FEED-FORWARD NETWORKS

This class of layered network differentiates itself by the presence of one or more hidden layers shown in the three-layer net, as shown in Figure 11.3. This network structure is referred to as a 3-3-2 network because it has 3 source nodes, 3 hidden neurons and 2 output neurons. The network shown in Figure 11.3 is said to be fully connected, in the sense that every neuron in each layer is connected to every other neuron in the next forward layer. If some of the communication links between the neurons are not part of the designed network, then it is referred to as partially connected.

The "hidden layers" communicate with the input and output layer in some purposeful manner. By adding a hidden layer or two, the neural net can handle some highly non-linear problems that would be complex to describe mathematically.

The best number of hidden layers depends on:

- the number of input and output units;
- the number of training cases;
- the amount of noise in the targets;
- the complexity of the function or classification to be learned;
- the architecture;
- the type of hidden layers activation function;
- the training algorithm; and
- regularisation.

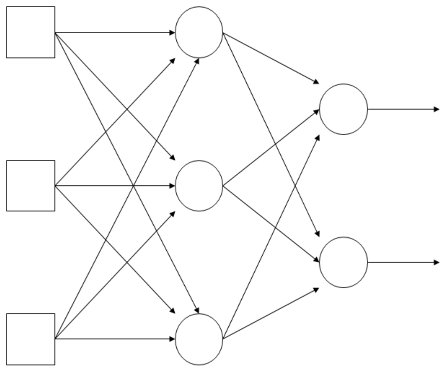


Figure 11.3: Fully connected feed-forward network with one hidden layer

If too few hidden layers are used, a higher training error and higher generalisation error will result due to under-fitting and high statistical bias. If too many hidden layers are utilised, a lower training error may be experienced, but with a higher generalisation error due to over-fitting and high variance [11].

However, from practical experience, it is known that little is gained by adding more than one hidden layer to a network, or if the net is too large, it will memorise rather than learn.

5. TRAINING A NEURAL NETWORK

An important task for a neural network is to learn a model of the application in which it will be operating, and to maintain the model adequately and reliably with the action of the real application, so as to achieve the particular goals of the application of interest [7].

So we see that training is as essential for a neural network as programming is for a computer to function properly. The correct choice of a learning algorithm is an important issue in network development. "Learning" means that the individual neuron's input/output behaviour changes as a result of changes in its local environment. The activation function of a neuron is fixed when the network is set up and the set of signals to which it is supposed to react is fixed; the only adjustment that can be made is to its weights and bias corresponding to the input vectors [13].

For different network structures, different training algorithms have been developed. Neural nets are classified according to their corresponding training algorithms: fixed weight networks, supervised networks and unsupervised networks. No learning is required for a fixed weight network, so common learning modes are supervised and unsupervised learning.

Supervised learning

The mainstream of artificial neural network development has been supervised learning networks. To commence learning, data needs to be gathered and consists of many pairs of input/output training sets. The sets of data are presented to the network, and through comparison at the output stage, adjustments of the weights and biases of the whole parameter space are made. In this way, learning or proper classification is facilitated with the help of a teacher, as shown in Figure 11.4.

Typically, simple perceptrons, feed-forward networks, need a teacher to tell the network what the desired output should be [14].

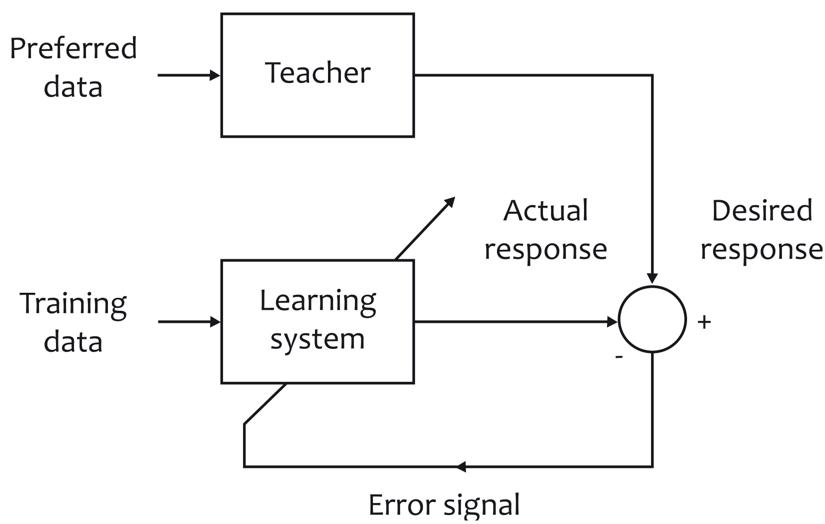


Figure 11.4: Block diagram of learning with a teacher

6. GENERALISATION

Once a number of training sets have been presented to the neural network, it is usually tested by feeding the neural network inputs that are not in the training set. In this way, it can be seen if the same output values in the training sets are approached when new, unknown input values are given. In this way, it can be seen how well the network will classify new, but not unrelated, input vectors or data sets.

A neural network can generalise when it correctly classifies input values that are not in its training data sets. A neural network can generalise well when the accuracy of classification is high, and vice versa.

An example of what generalisation might be is to compare it to curve fitting in statistics. When one attempts to fit a straight line to a fairly large amount of random data, and the data is well captured, there is confidence that an underlying relationship is captured in that data. Values of new data points not worked with in the fitting process can now be estimated using the fitted curve. If the straight line does not fit the data well, then another approach has to be taken (for example by using other new data sets or perhaps another statistical method).

Neural networks work in a comparable way. A complex, non-linear function is programmed by the neural network from its inputs. If the training data is fitted well by the trained neural network, and it classifies its data rather accurately, then there is probably some well-established mathematical relationship between the input/output vectors. Estimating outputs from new inputs would probably be more accurate now and it will be said that the neural net is generalising quite well.

For good generalisation:

- the number of training input vectors must be larger than the number of variable weights [15]; and
- the size of the weights rather than the number of weights determines the proper generalisation of the network [7, p. 111].

7. METHODOLOGY

The prediction of local electrical load at a source voltage of 132 kV is significantly more difficult than the prediction of bulk load at higher voltages, which exhibits a stronger statistical pattern due to an averaging effect. Most published papers on load forecasting usually deal with bulk load and can therefore give a fairly accurate prediction report.

For this study, electric load data was obtained from the 132kV voltage source at Harvard substation. This was used to develop an artificial neural model to accurately predict power demand with lead times ranging from half an hour to a week. This was required for planning of local load management in order to meet the expected demand.

A data range of local half-hourly *power demand* from which to train, test, and validate the different neural models was obtained to identify the *historical period* to be used [1]. Due to the rapid economic growth of the Mangaung Municipal area, older power demand data is of decreasing relevance as it does not accurately reflect the changes in the composition of the current load demand.

7.1 Gathering, processing and analysis of historical data

Historical load demand data for the years 2004 to 2007 from Parkwest Feeder 1 & 2 at Harvard 132 kV substation was obtained from Eskom, Bloemfontein.

HARVARD 132 kV SUBSTATION

LOAD DATA FROM PARKWEST FEEDER 1 & FEEDER 2

Recorder	Date	Time	kW	kvar	kW	kvar	TOTAL Kw	TOTAL Kvar	Recorder
"BF-00000000673	7/1/2006	30	78720	10560	72960	9600	151680	20160	"BF-00000000675
"BF-00000000673	7/1/2006	100	74880	9600	69120	8640	144000	18240	"BF-00000000675
"BF-00000000673	7/1/2006	130	72960	9600	67200	7680	140160	17280	"BF-00000000675
"BF-00000000673	7/1/2006	200	71040	8640	66240	8640	137280	17280	"BF-00000000675
"BF-00000000673	7/1/2006	230	70080	8640	64320	8640	134400	17280	"BF-00000000675
"BF-00000000673	7/1/2006	300	69120	8640	64320	7680	133440	16320	"BF-00000000675
"BF-00000000673	7/1/2006	330	70080	9600	64320	9600	134400	19200	"BF-00000000675
"BF-00000000673	7/1/2006	400	69120	8640	63360	8640	132480	17280	"BF-00000000675
"BF-00000000673	7/1/2006	430	70080	8640	64320	8640	134400	17280	"BF-00000000675
"BF-00000000673	7/1/2006	500	71040	7680	66240	7680	137280	15360	"BF-00000000675
"BF-00000000673	7/1/2006	530	73920	8640	69120	8640	143040	17280	"BF-00000000675
"BF-00000000673	7/1/2006	600	76800	8640	71040	7680	147840	16320	"BF-00000000675
"BF-00000000673	7/1/2006	630	82560	9600	76800	8640	159360	18240	"BF-00000000675
"BF-00000000673	7/1/2006	700	89280	11520	82560	10560	171840	22080	"BF-00000000675
"BF-00000000673	7/1/2006	730	96960	12480	89280	10560	186240	23040	"BF-00000000675
"BF-00000000673	7/1/2006	800	104640	13440	96960	12480	201600	25920	"BF-00000000675
"BF-00000000673	7/1/2006	830	114240	17280	105600	14400	219840	31680	"BF-00000000675
"BF-00000000673	7/1/2006	900	119040	19200	111360	16320	230400	35520	"BF-00000000675

7.2 Data pre-processing

Data pre-processing was done in three phases:

- Selected data was transformed to files in the EXCEL format to make importing and exporting the data to Matlab more efficient.
- Outliers and missing data were identified and discarded or rectified using statistical methods.
- Data entering the Matlab environment was normalised to the range [-1; +1] for the **A**rtificial **N**eural **N**etwork (ANN) to facilitate training and prevent "squashing" by the activation function [2].

7.3 Designing the ANN architecture

The ANN architecture was designed using the following criteria:

- Number of INPUT nodes
- Number of HIDDEN nodes

- Number of HIDDEN layers
- Number of OUTPUT nodes
- Interconnection of nodes
- Activation functions used in each layer

7.4 Training the neural network

A neural network model was constructed and trained for the four weeks of each month of the year for two previous years, as shown in Figure 11.5.

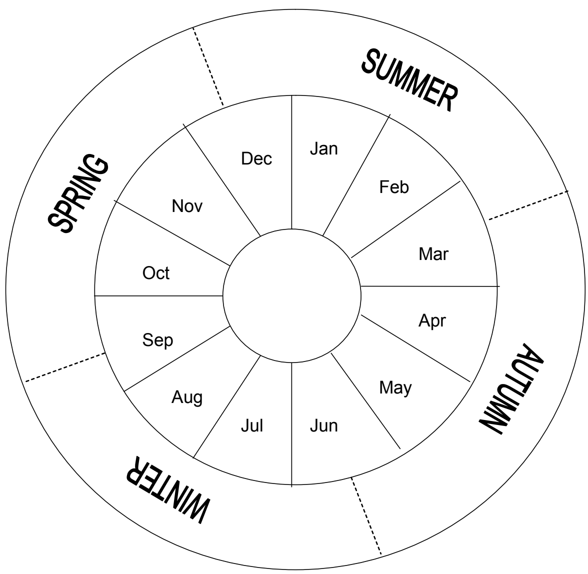
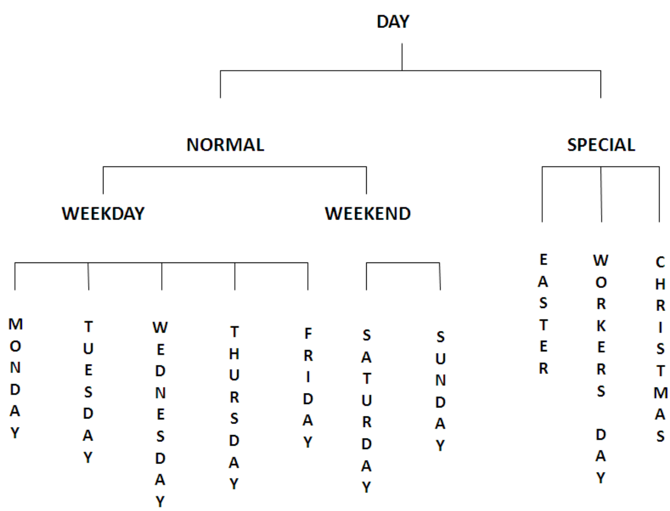


Figure 11.5: Segmentation of the forecasting model



Training of the neural network would involve the following actions:

- Different training algorithms would be tested for optimal speed and accuracy.
- The training parameters would be evaluated.
- Regularisation or "early stopping" was used to generalise the training model.

7.5 Application of the neural network model

7.5.1 Time series prediction with artificial neural networks

Time series methods are based on the notion that the data have an internal composition, such as autocorrelation or seasonal variation. A time series can be described as a chronological set of data measured over time, such as hourly, daily or weekly available data. The structure of this data set is then explored using a time series prediction method.

Artificial neural networks have been extensively used as time series predictors: these are usually feed-forward networks which make use of a sliding window over the input data sequence. The number of simultaneous data points taken, generally dictates the maximum resolution of the mathematical model. It is not always the case that the model with the highest resolution has the best predictive power.

This time series prediction is done using the half-hourly load data (discrete data points) as the only input parameters.

As an example, Figure 11.6 shows a back propagation neural network using four equally time spaced discrete data points to predict the next output data value on the graph.

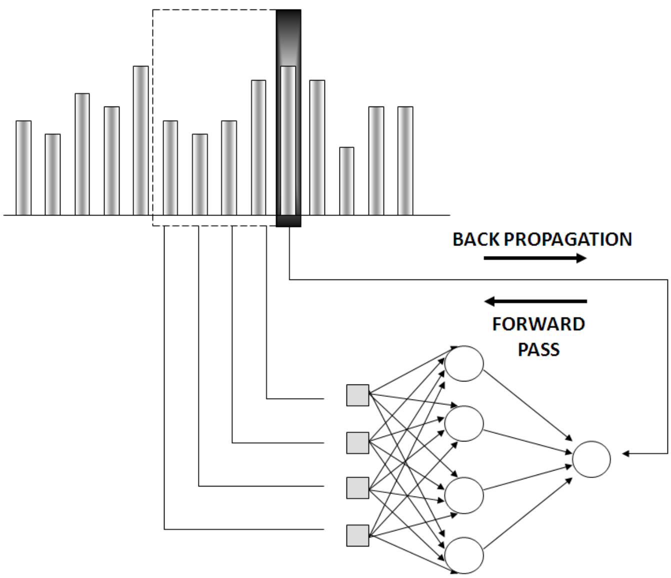


Figure 11.6: Time series prediction using the "sliding window" approach

A *4 to 36 step ahead time series predictor ANN model* was developed, tested, and validated, using the Mangaung-Bloemfontein real load data for certain months of the years 2004 to 2007 [12]. The accuracy of the predicted results produced by the neural network's outputs and targets was to be compared with actual, measured values, using statistical methods of regression analysis.

This would enable the use of future load data – to be obtained from Eskom – for the verification of the correctness of the modelled predictor.

8. RESULTS

A concatenating forward neural network was trained for week 1 to week 4 in June 2006, using the Levenberg-Marquart training algorithm. This network was then used to predict the half-hour ahead load in week 1 to week 4 in June 2008. Figure 11.7 shows the actual and predicted results of week 3 in June 2008.

The time horizon used was half-hour intervals. Twelve data points were used in the input representation and the logarithmic sigmoid function was used in the hidden layer.

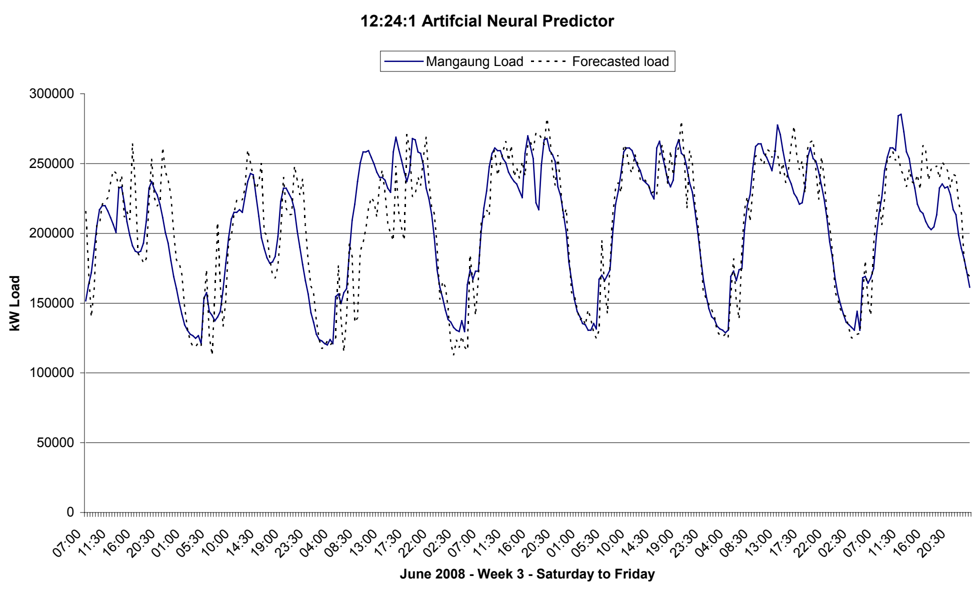


Figure 11.7: Actual and predicted load values using the neural forecaster

9. CONCLUSION

An extra short-term load forecasting model was developed, using a suitable artificial neural network with an appropriate back propagation training algorithm.

This model produced an extra short-term forecast of the load in 168 hours of any given week of the year, provided that it was trained and tested correctly. The technique was tested and validated on data provided by the Eskom power utility for the municipality of Mangaung, during 1994 to 1998. The predicted results, obtained through the application, showed that the ANN approach produced an efficient estimator.

Artificial neural networks are possible solutions and important approaches to short-term load forecasting. The functioning of sliding window feed-forward neural network predictors might be improved using theoretically observed heuristics.

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CHAPTER 12

Examples of Modelling Used in Modern Research

Ulrich D Holzbaur and Gerrit Jordaan

Modelling is an essential tool in scientific work, and is important for all disciplines in both the natural and human sciences. The following is an overview of the use of mathematical modelling in a variety of fields of study.

1. MATHEMATICS AND STATISTICS

Mathematics is concerned with the formal aspects of mathematical models, on formalising the models, and on deriving methods for problem solving. Despite the saying that, "Engineers think that their equations are an approximation of reality, physicists think that reality is an approximation of the equations, and mathematicians don't care", mathematicians are also considering the applications of their theory – mainly in terms of generic models.

The success of mathematical models lies in their applicability to all kinds of real world phenomena: The question by Albert Einstein, "Wie ist es möglich, daß die Mathematik, letztlich doch ein Produkt menschlichen Denkens unabhängig von der Erfahrung, den wirklichen Gegebenheiten so wunderbar entspricht?" (freely translated as: "How is it possible that mathematics, being a product of human thought independent from any experience, so perfectly describes the facts of the real world?"), can in part be explained by the fact that a lot of mathematical structures (e.g. geometry, algebra, analysis, topology) have been developed starting from real world problems.

Stochastics is – like mathematics – not only a science in itself, but also an important and mighty tool for research in various areas of science. Stochastic models can be mathematical models with a very sophisticated underlying theory or analogue, or iconic models with some intuitive (but sometimes misleading) understanding of probability, such as the model of Brownian motion. For potential pitfalls and failures in interpreting statistical results and probabilities, readers are referred to the Monty Hall Problem or books about "how to lie with statistics". These aspects are very important for research, and at all times care should be taken to prevent biased interpretation of test results.

2. NATURAL SCIENCE, ECOLOGY AND ENGINEERING

Best known are the mathematical models of physics. From elementary mechanics to quantum theory and relativity, physics and mathematics have influenced and stimulated each other. Dimensional analysis is a classic example of rather simple models. Any book on physics is concerned with models.

Models in ecology face rather similar challenges to those in economy and in geology. Some examples are given in [10].

In engineering, models serve as a description of the environment and the intended future use of the system in requirements analysis, and as a description of a possible future system. Product development can be seen as a series of model transformations from a requirement analysis through systems specification, design, drafts, and production models [4]. As computer programmes can themselves be seen as models in different ways (e.g. a model that can be executed by a computer, a model of what goes on in the computer, a model of some real world effects that have to be calculated, a model of the information a user is dealing with), the modelling process and the aspects of model transformation are even more important in computer science. An exemplary analysis of the importance of modelling and semantics in computer science is given in [3]. In the field of Artificial Intelligence, knowledge-based systems are explicitly based on models and their semantics.

3. ECONOMICS AND MANAGEMENT, AND SOCIAL SCIENCES

Models are a basis of economic theories and of operations research. Dynamic optimal decision models, or optimal control models, can be applied in any context that involves decisions, dynamics, and optimality criteria (e.g. the principle of economy). This applies to macro and micro-economics as well as to decision making in administration and military decisions on strategic, tactical, and operational level [7].

In economics and social science, we deal with very complex models that involve interactions between (groups of) human beings. Modelling processes, such as those for controlling behaviour, have to consider rebound effects from measures taken. As in quantum mechanics, the observation itself is changing the system, but unlike in physics, experiments in social science can hardly ever be repeated in a similar setting.

4. HISTORY AND GEOLOGY

With respect to modelling, history and geology have a lot in common. A challenging task for modelling is to display the four-dimensional movement of objects in a wide range of scales. In history, we consider the long-term migration of nations or short-term interactions between politicians or armies. In geology, we consider the movement of continents and tectonic plates, as well as the diffusion processes generating minerals or meteorite impacts. In addition, the objects (nations, continents) themselves vary in time and have a fractal or fuzzy structure. Here, as in physics, we have an easily modelled descriptive (kinematic) view or an explanative (dynamic) view that needs to consider a lot of interaction, forces and stochastics. As in economics, there is no experiment that can determine several alternative outcomes and strictly validate general "laws".

The difference in the models used in these two disciplines can be attributed to the difference in people and approaches between the humanities and natural sciences.

5. MODELLING OF MEDICAL CONDITIONS

Mathematical modelling also finds application in the study of medical situations.

MJ Blaser, a professor of Microbiology at the New York University School of Medicine, said: "We did not make the laws of nature. Even though we may not like them, we need to understand them to better control infectious diseases." This sentiment resulted in the development of a mathematical model – using game theory as developed by Nobel prize-winning mathematician John Nash – to study the interaction of microbes with humans, by Blaser and Denise Kirchner [10].

In summary, the results of the comprehensive modelling of the rules that govern the transmission of microbes indicate the probable evolution of particularly virulent microbes in future. This will be as a consequence of the increasing prevalence of HIV infection and an ageing world population, as well the growth in the world population. These results are the outcome of the scientific modelling of the laws of nature – as referred to by Blaser – as applied to a particular field of expertise, and it is now incumbent on the relevant authorities to monitor and manage the situation as it develops in future.

Collender described the use of mathematical modelling in the preparation for a possible influenza pandemic [2]. In particular, the cost of influenza for a modern economy has been studied, taking into consideration that 3000-4000 deaths occur every year in the UK due to flu, whilst it accounts for approximately 10% of sick leave in the USA with an estimated annual cost to the US economy of $10 billion. Therefore, it is clear that the incidence of influenza is a very costly and serious matter for any country, necessitating careful study and even, if possible, modelling of the phenomenon – especially of more serious strains such as bird flu.

A mathematical model has been developed correlating the UK's supply of antiviral drugs available – enough to treat 25% of the population – and the optimal way in which they can be utilised should such a pandemic actually occur. Several possible pandemic scenarios, with the appropriate drugs used at different rates, were modelled. It was found that the most effective strategy in mitigating the pandemic would be the quickest usage of the available stockpile – although it could lead to a depletion of the available resources.

Modelling always addresses the behaviour of a system as a consequence of the status of certain variables which have an effect on the system – the availability of a particular type of antiviral drug in the case above. However, such a study would normally include matters such as the availability of suitable national surveillance systems, levels of funding, quality of the health workforce, and the availability and implementation of appropriate health policies [6].

A further example of the use of mathematical modelling of medical conditions is that of the human cardiovascular system in the presence of stenosis [8]. Sud *et al.* modelled the entire system, represented by a large number of interconnected segments, based on the finite element method. Model parameters were based on published data on the physiological and rheological properties of blood. Computational results showed the way in which blood flow is affected through various parts of the cardiovascular system by stenosis in different blood vessels. In this manner, an improved understanding of such a critical phenomenon was arrived at.

6. MODELLING IN EDUCATION FOR SCIENCE AND RESEARCH

Models and modelling can be used as a means of education on any level (see, e.g. Blum *et al.* [1]). Moreover, modelling itself is a competence that must be studied over the course of an academic career. The modelling skills acquired during the course of (academic) education can be structured along the general skills development of researchers [5]. Such skills include, but are not limited to:

- the use of notations and connecting such to real world phenomena;
- the analysis and use of notions for various concepts;
- the interpretation and use of available models;
- reflection on the relation between model and reality;
- determination of the parameters of a given model;
- integration of the notations from several similar models;
- the creation of new models as instances of a given generic model;
- the creation of new models from a given model class or by integrating existing models;
- reflecting on the modelling process and on the impact of model semiotics;
- deriving own models and comparing model classes; and
- derive own model types, classes or modelling methods.

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Modelling as Research Methodology was written for the scientist and student researching the (expected) functioning of systems under specified conditions. As such, it represents an introduction to the use of modelling in natural, human and economical sciences. The book is divided into two sections.

The first section illustrates the *universal nature of modelling as aid to the researcher*. More specifically, this section focuses on the following:

- The principles of mathematical and scale modelling.
- A model for the design and development of physical devices comprising of elements of different engineering disciplines.
- The need for data acquisition facilities - especially in those cases where physical modelling is utilised.

In the second section of the book, several *typical examples of modelling* are described. These include a variety of studies such as:

- Modelling of the performance of an industrial freezer.
- Human-environmental dynamics with respect to a hydrological model.
- The prediction of short-term electrical load demand.

The Editors:

Professors Jordaan and Lategan are experienced in the guidance and supervision of researchers. Collaboratively and individually, they study the management of the research process, as well as the optimisation of the efforts of teams of researchers working on extended, multi-faceted fields of study. This is the second joint publication edited by these two individuals, on the topic of modelling as a research methodology.

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