1

Basic notions of modelling

1.1 MODEL, OBJECT, PHENOMENON

As in everyday language, so in science, the term **model** has many different interpretations. This term can be used by physicist, who speaks about a model of an atom or about a molecular interaction model, and by a chemist, who speaks about a chemical compound model, while an astronomer speaks about a model of the solar system. The same word, 'model' is often used in mathematics, biology, economy, sociology, geology, cybernetics and many other branches of science and technology. The concept of the model proposed by specialists dealing with particular subjects may differ, but all of them will probably agree with the following quite general definition:

> *an object M will be called a model of the object or phenomenon P if M is able to replace P so that the investigation of M provides some information about P.*

In the above definition we have used two words which seem worth detailed explanation. These are **object** and **phenomenon**. For purposes of such explanation let us consider the following example:

> Let a cantilever elastic rod of uniform section as in Fig. 1.1 be given. Suppose that all the necessary geometrical characteristics (i.e. initial length l, cross-sectional area A) as well as material data (i.e. Young's modulus E, density ρ, coefficient of linear thermal expansion α, etc.) are known. We shall consider three phenomena in which the same object—the rod—takes part.

The first phenomenon under consideration is expansion of the rod due to a constant force F applied on its free end. We seek the extension of the rod. As we know, according to Hooke's law, extension of the rod is

$$\Delta l = \frac{Fl}{EA}. \tag{1.1}$$

Consider now a second phenomenon involving the same object. Let us now suppose that instead of the constant force F, a time-dependent force $F(t)$ is applied to the free end of the rod. Again we seek the displacement of a given cross-section of the rod, particularly that at its free end. Since our immediate task is only to illustrate some ideas and not

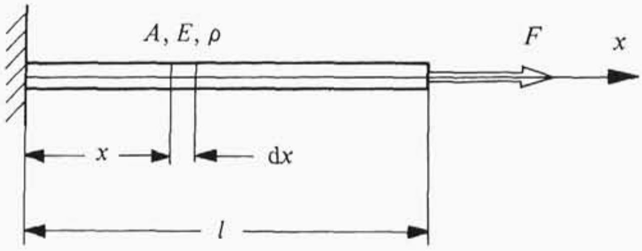

Fig. 1.1.

to deduce the equation of longitudinal vibrations of the rod nor to solve it, we shall only quote it below. Thus the model of the longitudinal vibration of the rod is (see for example Meirovitch (1967)):

$$\frac{\partial^2 u(x,t)}{\partial x^2} - \frac{1}{c^2}\frac{\partial^2 u(x,t)}{\partial t^2} = F(t)\delta(x-l), \tag{1.2}$$

where δ is the **Dirac function**, $c = \sqrt{(E/\rho)}$ is the wave propagation velocity, and ρ is the mass density.

The solution of (1.2), i.e. the displacement $u(x, t)$ of the cross-section given by coordinate x, has the following form:

$$u(x,t) = \frac{4c}{\pi EA}\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{2n-1}\sin(2n-1)\frac{\pi x}{2l}\int_0^t F(\tau)\sin(2n-1)\frac{\pi c}{2l}(t-\tau)\,\mathrm{d}\tau. \tag{1.3}$$

The displacement of the free end of the rod can be obtained by substituting $x = l$ in (1.3). Thus we have

$$u(l,t) = \frac{4c}{\pi EA}\sum_{n=1}^{\infty}\frac{(-1)^{n-1}}{2n-1}\sin(2n-1)\frac{\pi}{2}\int_0^t F(\tau)\sin(2n-1)\frac{\pi c}{2l}(t-\tau)\,\mathrm{d}\tau. \tag{1.4}$$

A further simplification of the general result (1.3) may be obtained if we assume a particular form of the excitation force $F(t)$, and if we additionally reduce the number of terms of the infinite series appearing in solution (1.4). For the force in the form as in Fig. 1.2, i.e. $F(t) = F_0 1(t)$, where $1(t)$ is the so-called **unit step function**, and taking into account only the first term of the infinite series, i.e. $n = 1$, we get

$$u(l,t) = \frac{Fl}{EA} - \frac{8Fl}{\pi^2 EA}\cos\frac{\pi c}{2l}t. \tag{1.5}$$

Comparing (1.1) and (1.5) we can easily note a difference between a static extension of the rod and its dynamic behaviour under time-varying force excitation.

Finally let us consider a third phenomenon involving the same subject—the rod. Suppose that the temperature of the rod has been increased from 0°C to θ°C. We ask now about the expansion of the rod due to change of temperature. We know from physics that

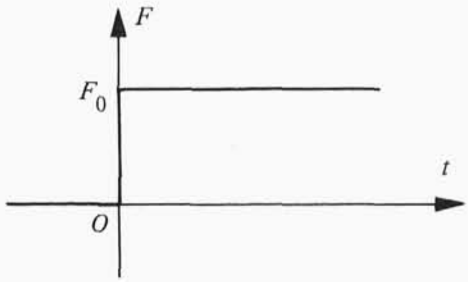

Fig. 1.2.

$$\Delta l = l_0(1 + \alpha\theta), \tag{1.6}$$

where l_0 is the initial length of the rod in temperature 0°C.

The above example shows that the same object, the rod, may appear in three different phenomena. Consequently, we have to distinguish the notions of *object* and *phenomenon*. Moreover, we may suspect that a model of the phenomenon, rather of the object, is usually important.

In the examples considered we have dealt with an object, the rod, as a certain real thing. However, the word object is used in two slightly different meanings. Usually we have in mind a real thing like an aircraft, a car, a bridge, a ship, a cloud, a river, but we would also include simpler things which themselves may be considered as models, such as a particle, a rigid body or a deformable body. But sometimes the word object is used to denote an abstract entity such as a system of equations or a mathematical relation. Thus we shall distinguish the narrow and the wide meanings of the word 'object', the wide one including both real and abstract meanings. It is in the wider sense that the word object has been used in the definition of the model. A real object or phenomenon P may be modelled by means of any other real object M_1 or also by means of a set of equations of motion M_2.

The examples considered show that for the same object different kinds of phenomena may occur. The specific phenomenon occurring depends on the type of excitation applied.

The relation between the object and the phenomenon may be also explained by means of a cybernetic scheme of a system (Fig. 1.3). Acting on the object, the input signal x, i.e. *excitation*, causes a certain time–space process. Some variable parameters of the process may be regarded as the output signal y, i.e. the *response*. For example, displacements of the object elements or forces exerted by any part of the considered object on another

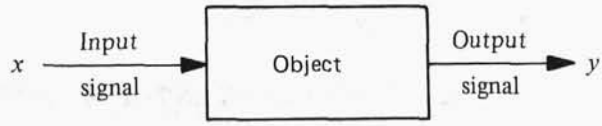

Fig. 1.3.

object may be regarded as output signals. We shall call a phenomenon one of any possible realizations of the time–space process occurring within a certain system.

Let us now further explain the notion of 'model'. The definition given comprises two different interpretations of the word 'model' used in engineering sciences. In the first, a model is a device which, by replacing a real object, gives information about the real object or its behaviour during a phenomenon. Such a device, usually of reduced dimensions, is useful for the modelling of a phenomenon, whose investigation would be too expensive or even impossible if performed on the object at natural scale. Models of this kind are often used in the aircraft and ship industries. Another, non-economical, reason for constructing devices serving as models is the lack of adequate mathematical description of certain real phenomena. An example of such a phenomenon is atmospheric turbulence. It is these aspects of modelling, i.e. how to build such models and how to plan experiments, in which the model behaviour may give crucial information about a real object, that has necessitated the development of similarity theory (Sedov (1982)).

The words 'model' and 'modelling' are often used in engineering sciences to denote a mathematical description of the investigated phenomenon and the process of forming such a description, respectively. This second meaning of the words 'model ', and 'modelling' will be our subject of interest, and the terms will have only this meaning in what follows.

Thus, modelling seems to be an activity that engineers need. To explain the status of modelling among other groups of engineering activities we shall consider the following scheme (Fig. 1.4). The three circles represent the *real object*, its *mathematical model*, and a *new object* (which, for example, is to be designed), while the triangle represents *properties* of the object. Suppose that we need to determine a certain group of properties of the real object or its behaviour under a certain excitation. Two different procedures are possible. The first is direct *measurement*, while the second requires a formulation of the mathematical model, and then its *analysis*. By means of this indirect way, via *modelling* and analysis of the model, interesting properties can be determined. Now suppose that a design problem has been stated, i.e. a new object which fulfils a group of requirements has to be constructed. In this case, too, in general, there are two possible ways of constructing the new object. The first, called *experimental synthesis*, relies upon reconstruction or modification of consecutive, improved objects until the required properties are achieved. During this process the results of previous experiments are continuously used. The second approach has many variations, but all of them refer to the mathematical model and all of them use calculation techniques. Therefore we shall call this approach *calculational synthesis*. This group of activities encompasses, for example, modifications based on sensitivity theory. Thus modelling is one of the five main activities of engineers. Many excellent books have been published on measurement techniques, different methods of analysis or particular synthesis techniques. Very few, however, are devoted to the art of modelling. We hope to fill this gap to some extent.

1.2 INVESTIGATION OF PHENOMENA BY MEANS OF MODELS

There are two main ways of formulating mathematical models. The first, theoretical in principle, is based on direct application of physical laws, while in the second, the

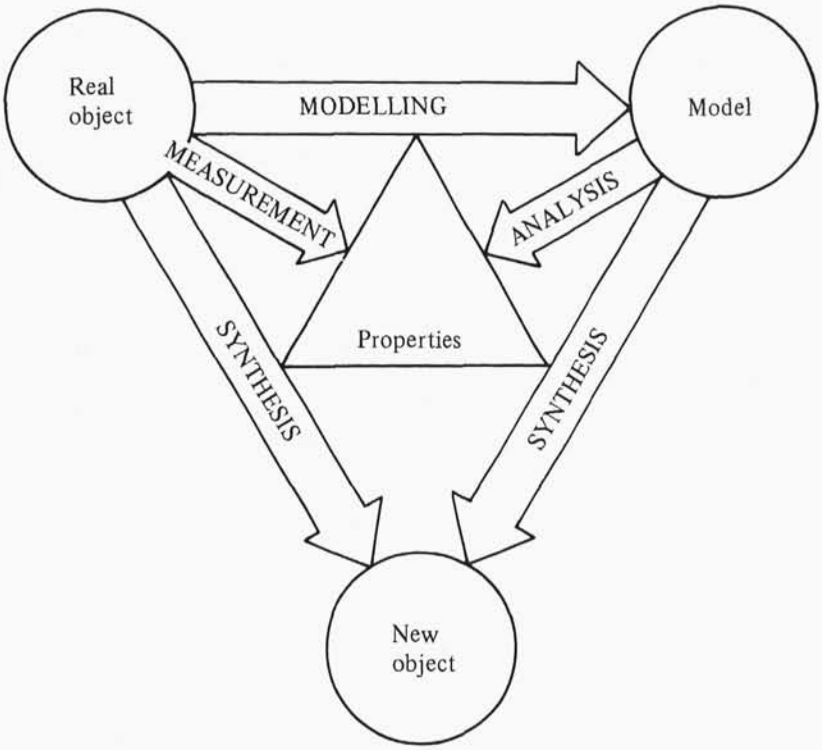

Fig. 1.4. A scheme of engineering activities.

fundamental role is played by the experiment. We shall give an outline of both methods in this section.

1.2.1 Physical modelling

The elements of modelling we dealt with during our school days were meant for solving of problems of the following kind:

> a boat travels on a river between towns A and B which are 20 km away from each other; let the river velocity be $u = 5$ km/h, and the velocity of the boat in calm water be $v = 15$ km/h; assuming that the boat's engine works constantly with the same power, calculate how long it takes to go from A to B and to return to A.

The problem given above shows a situation that is in fact far away from reality. We have not taken into account many aspects of a real event which may have in reality taken place. We have omitted, for example, such elements as air temperature, wind velocity, momentary changes of river velocity and many others. A question arises: why is the information given in the problem only a subset of the complete set of information related to a phenomenon? The kind of objects taking part in the phenomenon and the aim of the modelling process have crucial significance for determination of the necessary subset of information, enabling us to solve the given problem. In the case considered the question is 'how long does the progress of the boat up and down the river between places A and B take?' This particular question calls for a certain amount of information which has to be contained in the description of the phenomenon. No factors of the real event are included unless they have some influence on the duration of the journey.

Let us now consider another phenomenon which may occur on the same river. Suppose that in a town A an ecological catastrophe had taken place due to which the water was polluted. We ask how long would it take for polluted water to reach town B situated, as we remember, 20 km downstream from the pollution source A.

Let us note that although the question is similar to the one in the first example, the moving object is different. This time it will be significant whether the polluting substance dissolves in water, and what is the wind direction and velocity, which in the case of a substance floating on water, such as oil, would influence the speed of pollution advance.

Suppose now that the aim of modelling has been given. The activity based upon the distinction of substantial elements of the phenomenon considered, i.e. establishment of

— qualitative features and quantitative characteristics of excitations and responses, i.e. input and output signals, respectively,
— qualitative features and quantitative characteristics of the object,
— assumptions simplifying excitations and the object itself, and
— physical laws governing the phenomenon.

is called **physical modelling**.

The effect of this stage of the modelling process, i.e. a set of mathematically non-formalized pieces of information concerning the phenomenon, will be called a **physical model**.

Two expressions, *qualitative feature* and *quantitative characteristics*, used in the above definition seem to be worth a short explanation. Speaking about qualitative features we have in mind such possibilities as

— linearity or nonlinearity of the object elements,
— discrete or continuous nature of the object elements,
— discrete or continuous operation of input (output) signals,
— invariability or variability of the object elements,
— deterministic or probabilistic character of the object parameters,
— deterministic or probabilistic nature of the input (output) signals.

Then, determination of quantitative characteristics is connected with

— determination of the measures for quantitative description of the object elements as well as input (output) signals,
— performing proper measurements of input signals and all physical parameters of the object elements that influence the behaviour of a system.

For the heuristic purpose of easy memorization we can employ a short definition of the physical model, namely that it is a **graph and causa efficiens**. This should be understood in such a way that a physical model consists, as a rule, of a scheme of the device or object (that is a graph), the list of simplifying assumptions, and the list of physical laws governing a given phenomenon (that is, *causa efficiens*).

Since a physical model is a simplification of a certain reality, the real phenomenon differs from the one resulting from a physical model. To distinguish, in what follows, between the real and the simplified phenomenon, which results from the physical model, we shall call them simply **phenomenon** and **event**, respectively, i.e. an event is a phenomenon simplified by assumptions made within the framework of a physical model.

According to the physical modelling definition, the physical model is only a simplified reflection of the reality. Thus a model is not just the sum of our knowledge about a phenomenon. A model should represent that part of our knowledge about the phenomenon which is important with respect to its purpose. Taking into account the above remarks, we have to be aware that the decisions undertaken at the physical modelling stage have a crucial influence on the form of the mathematical model. For this reason the determination of qualitative features of the object elements and input signals should be done with particular care and with awareness of the consequences of this or another choice.

1.2.2 Mathematical modelling

Suppose that a physical model has been established. The next stage of modelling, resulting in the determination of a mathematically formalized description of the event, will be called **mathematical modelling**. The result of this stage of modelling, i.e. a set of equations together with initial, boundary, and signal value range conditions, will be called a **mathematical model**. Thus the general form of a mathematical model of a phenomenon is

$$G(\tilde{x}, \tilde{y}) = 0, \quad \tilde{x}(t_0) = \tilde{x}_0, \quad \tilde{x} \in X, \tag{1.7}$$

where $\tilde{x}$ is a mathematical description of real input signals x, $\tilde{y}$ is a mathematical description of real output signals y, G is an operator acting on functions $\tilde{x}$ and $\tilde{y}$, and X is a set of functions describing input signals.

Mathematical descriptions of input and output signals $\tilde{x}$ and $\tilde{y}$, are, generally, functions of time and space coordinates. The form of the operator G depends on qualitative features and quantitative characteristics of the object but first of all depends on physical laws governing a given phenomenon.

If the form of the operator G enables a solution of the equation (1.7) with respect to $\tilde{y}$, then we may write

$$\tilde{y} = L\tilde{x}, \tag{1.8}$$

and then the operator L may be called the **mathematical model of the object**.

The phrase 'a model of an object', e.g. 'a model of an aircraft', is commonly used among engineers, without specifying whether it concerns a physical model of that object or a mathematical model of its behaviour in flight, i.e. a phenomenon in which a given object participates. In most instances the meaning of this phrase is clear from the context. In this book, however, we shall deal only with modelling of dynamic processes and therefore when the word 'model' is used it refers, usually, to a mathematical model of the phenomenon. In those cases when the phrase 'a model of an object' is used, we have in mind, as a rule, a physical model of that object.

There is one more thing that seems to be worth explaining now. The notion of 'mathematical model' encountered in the literature refers to equations like (1.2) as well as to expressions which are usually solutions of equations, such as (1.3)–(1.5). We shall distinguish these two groups of mathematical relations and we shall call a **proper mathematical model** (or simply a mathematical model) an equation, usually differential equation, relating excitations to responses. Solutions of these equations, i.e. functions relating responses to excitations, will be called **resulting models**.

Thus, one can say that the complex process of modelling could be summarized in the form of the following problem: determine such an operator G that for all input signals x from a certain range, their mathematical models $\tilde{x}$ cause output signals $\tilde{y}$ to imitate sufficiently well respective signals y.

1.2.3 Identification as a method of model formulation

Considerations of sections 1.2.1 and 1.2.2 may suggest that the determination of a mathematical model is always preceded by the construction of a physical one. Is this the only way for mathematical models to be formed? Before we shall answer this question let us consider some aspects of complex technological processes, such as, for example:

— ammonia synthesis,
— oil distillation, or
— glass melting.

It happens very often that such processes have to be automatically controlled by means of a computer, or the properties of a final product should be improved or even optimized. For these reasons a mathematical model is required. But in the case of complex technological processes some or even a majority of physical model components are unknown. Knowledge about physical or chemical laws governing a given process is incomplete. Another source of incomplete information is constituted by input signals, which can be divided into three groups:

— control signals, which enable influence to be exerted on the course of a technological process,
— disturbance signals which can be directly measured, and
— disturbance signals which cannot be directly measured, and these are the sources of incomplete knowledge about the phenomenon.

A good example of this kind of situation is provided by modelling of the glass melting process. Suppose that we would like to know how certain properties of glass, such as colour, coefficient of thermal expansion or elastic constants, depend on the composition of the mixture from which glass is made, or on the characteristics of a technological process like the time–temperature relation of heating, melting, cooling and hardening processes. The mathematical model should comprise relations between the interesting output properties of glass and the input parameters which, in the case considered, are proportions of the mixture components and parameters of the whole melting process.

Physical and chemical laws, however, accompanying the melting process are not known to such an extent as to be a basis for writing down the interesting relationships between input signals of the process and output properties of glass. Nevertheless, the mathematical model of glass properties can be formulated. The procedure leading to the model consists of the following steps:

(1) carrying out of a series of experiments with careful measurement of input signals, parameters of the process itself and output properties;
(2) formulation of assumptions concerning the general form of the model (for instance, linearity of the model, the order of system equation, etc.);
(3) computational determination of all the assumed model coefficients; this step may be performed by means of a computer, using such techniques as regression analysis, factorial analysis or component analysis.

This experimental–calculational procedure of mathematical model formulation is called **identification**. The procedure described provides an alternative way of mathematical model creation. Let us summarize the typical features of an identification procedure:

— lack of some or all elements of a physical model,
— use of experimental data,
— computerized calculation of the final form of the model.

1.2.4 Investigation of the mathematical model

Mathematical model creation does not complete the process of investigation of a phenomenon. Usually the next step is the **investigation** of the model, i.e. its analysis. For the task of model investigation a variety of methods may be applied. However, since it is analytical solutions that are most desired by the scientists, analytical methods of investigation of the model are essential. Examples of this kind of solution have been considered in section 1.1 (see, for instance, relation (1.3) for the mathematical model (1.2)). The analytical form of solutions usually provides the largest amount of information about the evolution of the phenomenon. We aim, therefore, as a rule, at obtaining analytical solutions. However, the complexity of many physical processes makes it difficult or even impossible to obtain solutions in analytical form. In those cases, approximate or qualitative methods may be useful, but in many cases computer simulation methods may be applied.

There are numerous methods of mathematical model analysis and also of computer simulation. Many, or even perhaps a majority, of engineering texts are devoted to different aspects of model investigation, i.e. to the analytical solution of equations or to computer simulations. We shall not follow this path and, as a rule, we shall concentrate in this book on the problem of mathematical model formulation. In some cases in which, for different reasons, solution of a model will be required, it will be quoted rather than derived.

1.2.5 Verification of solutions

Attempts should be made to validate the model, that is to check whether the theoretical solution is in good agreement with the observations from the real situation. If there is good correlation, then the model can be used either to give a theoretical explanation for the observed phenomena, to predict further results, or to help in making decisions. On the other hand if the correlation between the theoretical and observed results is not adequate, we must return to the assumptions made at the stage of physical modelling and decide which need modifying or what additions should be made. The cycle is then traversed once more to see if the new model gives an adequate description of the real problem.

This stage of investigation of the phenomena by means of models is closely connected with the modelling purpose assumed at the very beginning of the modelling process. The term **solution verification** will be understood not only as a comparison of mathematical model solutions with the evolution of the phenomenon, but also as an evaluation of the model formulated made from the point of view of realization of the modelling purpose. After such an evaluation the model may turn out to be

(1) **adequate**, i.e. simply **good**, if its solutions give the answers to all interesting questions with required exactness and the model itself is the simplest possible one,
(2) **inadequate**, if the model does not fulfil the requirements of model adequacy. We shall distinguish two types of inadequate models:
    (a) an **incomplete model**, i.e. one that may become adequate after it has been supplemented.
    (b) an **excessive model**, i.e. one that can become adequate via its simplification.
(3) **wrong**, if passage to the adequate model is linked with a substantial change of a physical model.

1.2.6 Investigation of the phenomena—summary

The complex process of investigation of phenomena may be schematically illustrated by means of notions from set theory. Let us introduce the following four sets:

— R, whose elements r_i are real objects or phenomena,
— P, whose elements p_i are physical models,
— M, whose elements m_i are mathematical models, and
— S, which elements s_i are solutions of the mathematical models.

Now we are in position to discuss Fig. 1.5. The four circles marked by R, P, M, S respectively represent the sets introduced above, while the broad arrows represent the five main activities of the investigation process. The picture shows that there is no unique relationship between the elements of different sets. This is easy to accept, knowing that the same physical model may represent different phenomena and vice versa, i.e. a given phenomenon, when modelled according to different modelling purposes, may result in different physical models. Similar situations appear for successive pairs of sets and this fact is reflected in Fig. 1.5. Additionally, let us note that not every physical model p_i has its counterpart in the set M of mathematical models, and not each mathematical model m_i has its solution within the set S. As well as continuous lines there are also broken lines. These show the influence of respective modelling stages on the previous ones. It often happens that certain observations, results, or even difficulties encountered at the subsequent stages imply necessary modifications of previous results. Thus, all these activities

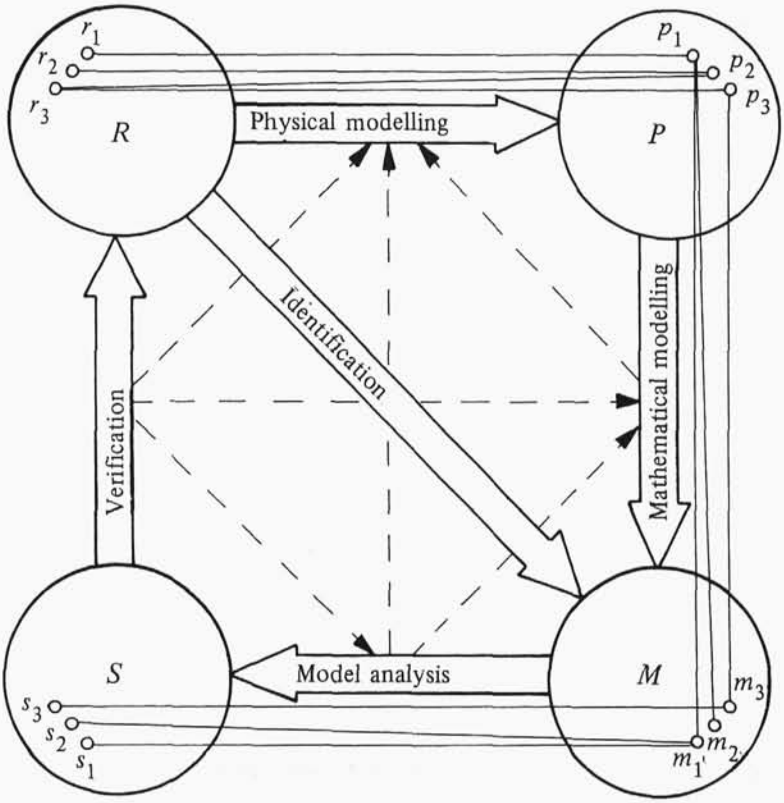

Fig. 1.5. Scheme of the process of investigation of the phenomena.

which are symbolized by broken lines will be called **modifications**. It should be stressed that in practice most modelling does not take the precise form shown in Fig. 1.5. The figure is there just to give some idea of the underlying relationship between real-world problems and the mathematical techniques used to find solutions to them.

1.3 AN EMPIRICAL AND A CAUSAL MODEL

Each observed phenomenon may be described in many different ways depending on factors such as required exactness, the purpose of modelling, calculation possibilities at the stage of model analysis, etc. Even if all the mentioned factors have been established, two different approaches to mathematical model formulation may still be distinguished. These two approaches result in different kinds of models. However, before naming them let us consider an example in which two methods of mathematical model formulation will be presented.