Chapter 2
Systems Analysis: The Strategy of Modeling

Modeling is one of the most widely used methods for studying various systems. It provides a way to reveal qualitative and quantitative interrelationships between various parameters of the object of investigation.

Modeling begins with defining a subject of investigation, i.e., a system of concepts that reflects the characteristics of the object that are significant for modeling. The systems approach is generally used in the analysis and synthesis of large systems. Systems analysis is the strategy for studying complex systems that include objects and processes of diverse physical nature, whose functioning is described by a large amount of information. The following principal steps underlie systems analysis [1–3]:

- clear formulation of the goal of the investigation;
- statement of the problem in terms of achieving the goal and defining an efficiency criterion for solving the problem;
- development of a detailed research plan with indication of the principal steps and directions for solving the problem;
- systematic advancement along the entire set of interrelated steps of the research plan;
- organization of successive approximations and repeated cycles in the individual steps;
- application of the principle of a descending analysis hierarchy and an ascending synthesis hierarchy in solving the component particular problems.

A basic method of investigation used in systems analysis is mathematical modeling, and a basic principle is the decomposition of a complex system into simpler subsystems, i.e., blocks. Accordingly, models are constructed by the building block principle: the overall model is subdivided into blocks, to which a comparatively simple mathematical description can be given [1–3]. Application of the decomposition technique to the analysis and mathematical modeling of large

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technical systems, which are distinguished by a high degree of complexity and a multilevel structure, is especially effective [4–8].

Systems analysis is based on fundamental principles, whose fulfillment ensures the successful modeling and simulation of complex systems of diverse physical nature and information structure [9, 10]:

- the principle of a final goal—the absolute priority of the final goal;
- the principle of unity—combined consideration of the system as a whole and as a collection of interrelated parts;
- the principle of connectivity—considering any part of the system together with its connections to other parts and the surrounding environment;
- the principle of modularity—demarcating modules (blocks) in the system and consideration of the system as the complete collection of these modules;
- the principle of hierarchy—establishing the subordination of the modules;
- the principle of evolution—taking into account the variability of the system and its ability to evolve and store information;
- the principle of decentralization—combining the methods of centralization and decentralization in the solutions employed;
- the principle of indefiniteness—taking into account the indefiniteness and randomness in the system.

All of these principles are used in nearly any application of the systems approach. They have a very high degree of generality, but the existence of conditions under which any of the principles will be insignificant is possible in each particular case. For example, there may be no hierarchy in a system, which can be considered completely defined, etc. The practical implementation of these principles in the modeling of specific complex systems ensures the effectiveness of the models developed and optimization of the processes in the system. The use of these principles will be illustrated below in the modeling of objects and processes.

2.1 Methodology of Modeling

In systems theory a model is an approximate description of a system that reflects its specified properties, which are generally fundamental properties with respect to the modeling goal. The term model refers to a material or mentally represented object, which replaces the original object during a study, but maintains some typical features of it that are important for the particular investigation. A well constructed model is generally more accessible, informative, and convenient for the investigator than the real object. Investigations performed on models enable investigators to do the following:

- to understand how a specific object is organized and what its structure, fundamental properties, laws of evolution and self-evolution, and interactions with the surrounding environment are;

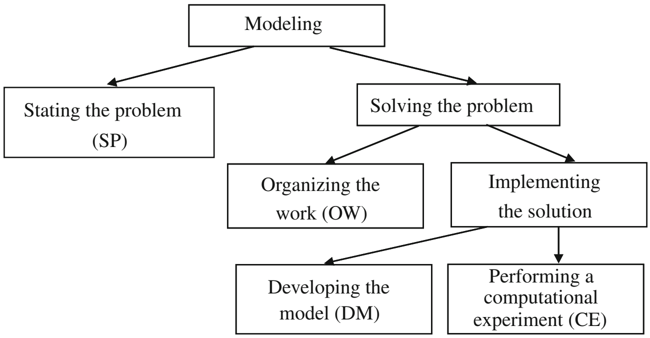

Fig. 2.1 Block diagram of the modeling process

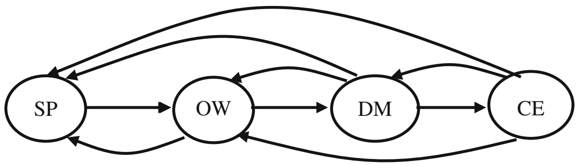

Fig. 2.2 Iterative nature of the modeling process

- to learn to control an object or process and to determine the optimal operating conditions for assigned goals and criteria;
- to predict direct and indirect consequences of the realization of assigned modes and forms of action on an object.

The methodology for creating models of complex systems can be represented in the form of a block diagram that reflects the sequence of the main stages of the modeling process (Fig. 2.1).

It should be noted that the modeling process has an iterative character, as a result of which the model that most faithfully describes the system under study is created. It is manifested in the continuous correction and modification of the model, which provide a way to obtain its optimal variant (Fig. 2.2).

We will consider each of the stages in the development of a model that are shown in Fig. 2.2 in greater detail.

2.2 Stating the Modeling Problem

The main goal of this stage is preliminary investigation of the modeling object and formulation of a meaningful (descriptive) statement of the modeling problem, which is generally not final and can be refined and made more specific during the development of the model. If the modeling object is a technological process or a

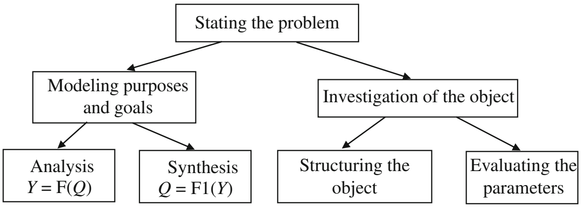

Fig. 2.3 Block diagram of the stage of stating the modeling problem

technical object, the meaningful statement of the modeling problem is very often called the technical statement of the problem. This stage includes the following operations:

- thorough inspection of the modeling object itself for the purpose of revealing the main factors and mechanisms that determine its behavior, as well as the parameters that allow description of the object being modeled;
- collection and verification of the existing experimental data for analogs of the object and performance of additional experiments when necessary;
- an analytical review of literature sources, analysis and comparison of existing models of the object or objects similar to it with one another;
- analysis and summarization of all the accumulated material.

We represent this stage of the modeling process in the form of a block diagram (Fig. 2.3). In the general case three principal modeling problems of complex systems can be distinguished: research, design, and control. From the theoretical point of view, research problems can involve obtaining new scientific knowledge, and from the applied point of view, they can involve optimization of technological processes. Designing refers to the creation of artificial man-made objects that have desirable properties. The control of processes or objects is possible, in particular, in the form of regulation and optimization. Depending on the problems posed, modeling goals that are uniquely related to data for performing research, design, or control are formulated.

Analysis and synthesis can be included among the basic goals of modeling.

Analysis is the calculation of the output parameters of a process from assigned values of input parameters. In other words, in analysis problems an evaluation is made according to the “What will happen if …?” principle.

Synthesis is the determination of the values of the input parameters of a process for which assigned values of the output parameters are achieved. In synthesis problems the question “What is needed in order for …?” is resolved. In this case the problem of determining the best operating conditions of a system can be solved, i.e., the modeling goal is optimization of the process.

A comparison of the problems and goals of modeling enables us to state that there is a correspondence between them. In particular, analysis is employed in research problems, synthesis is employed in design problems, and analysis and synthesis are employed together in control problems (Fig. 2.4). Modeling problems can be described in the form of target functions:

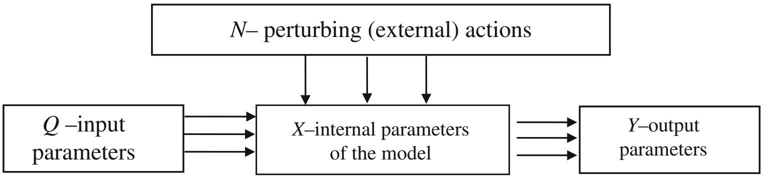

Fig. 2.4 Diagram of the purpose of modeling problems

- research: $Y = \mathrm{F}(Q, N, X)$;
- control: $Q = \mathrm{F1}(Y, N, X)$;
- design: $X = \mathrm{F2}(Q, Y, N)$;
- design with optimization of the parameters: $Q, X = \mathrm{F3}(Y, N)$.

When the properties of the object and resources available to the investigator are taken into account, the goals can be refined and corrected.

To achieve practical modeling goals, a need to consider the object under investigation not as something whole, but as a collection of separate interrelated elements often arises. In some cases this is specified by the complexity of the object of investigation itself, and in other cases it is due to the absence of necessary information about the object or appropriate mathematical machinery. The process of dividing a system into elements with indication of the connections between them is called structuring or decomposition. The division process can have a material, functional, algorithmic, or other basis. As a result of decomposition, the original system breaks down into subsystems, and the problem breaks down into subproblems that have known solutions or can be solved using approved methods. However, it is important not just to divide the whole into separate elements, but also to combine them in such a manner that they would again form a single whole. Therefore, analysis and synthesis methods are widely employed in this stage of the work. Analysis methods are used to divide the object under consideration into separate elements and study their properties. During decomposition, at least two criteria, namely completeness and simplicity, must be taken into account. Of course, some compromise between completeness and simplicity should be made during decomposition. This can be achieved if only elements that are significant with respect to the modeling goal are included in the structure of the system. The problem can be simplified by diminishing the inputs and outputs of each element in comparison to the original state. Accordingly, separate properties of the system as a whole and/or properties of its separate elements can be lost during analysis. Synthesis supplements analysis, since the correctness of the decomposition process can be evaluated only after all the elements have been added to the system. The synthesis process provides a way to join the elements to one another and to establish the relationship between them, i.e., to obtain a structural diagram of the object of investigation. The stable ordering of the system's elements and connections in space is called its structure. For example, a technological process is characterized by a definite sequence of technological operations in time, and a technical object is characterized by a definite arrangement of nodes and parts in space. A structural diagram represents the elements (blocks) and the order in which they are joined. Each element (block) is depicted by a rectangle, and the connections between them are depicted by arrows, which indicate the direction of action. A structural diagram graphically shows the existence of phenomena that occur consecutively and in parallel and closed loops caused by the presence of feedback in the system. The structure of the interaction of the phenomena allows well-founded selection of the ones that it would be expedient to include in the model. For example, phenomena that form a consecutive chain of connections between input and output parameters must be included in the model. The parallel phenomena whose contribution to the overall effect is small may be disregarded. Reverse connections can be disregarded if their strength is insignificant. Thus, rough quantitative estimates of the contributions of phenomena to the final result of the process are useful, and often necessary, for selecting the significant phenomena. The required accuracies of the modeling result and of the original data play an important role in selecting the phenomena that are taken into account in a model of a process. Obviously, a phenomenon can be disregarded only in cases where its contribution to the final result is smaller than the required modeling accuracy or smaller than the error caused by the inaccuracy of the original data.

In the general case parameters which describe the state and behavior of a modeling object can be divided into the following groups (see Fig. 2.4):

- the collection of input (controllable) actions on the object (Q);
- the collection of actions of the external environment (uncontrollable) (N);
- the collection of internal (intrinsic) parameters of the object (X);
- the collection of output characteristics (Y).

A description of each parameter and variable is given in the following form:

- definition and brief characterization;
- notation symbol and unit of measure;
- range of variation and accuracy of assignment;
- place where it is used in the model.

The number of parameters of all types in models is finite. Each of the parameters can have a different "mathematical" nature: it can be a constant or a function, a scalar or a vector, a crisp or fuzzy set, etc. Sometimes parameters can be assigned in the form of a qualitative characteristic. In the general case the following types of factors and interactions between them can be identified within a model [11, 12]:

- variables—factors that take arbitrary values, on which the behavior of the system or its state depends;
- parameters—factors that are taken into account in the model and can be set at fixed levels or according to assigned dependences;
- functional relations—equations that describe the interdependence between variables and parameters when the system functions;

- constraints—established limits of variation of parameter values or conditions that ensure a normal regime for the occurrence of processes in the system;
- target functions—parameters for optimization of the operation of the system, which must take extremum values to achieve the most efficient operating conditions of the system with consideration of the possible constraints, which depend both on the properties of the system and on its interaction with other systems and the environment.

To successfully construct a model, all of its parameters and variables must be considered, and their influence on the functioning process of the system as a whole must be evaluated. Isolating the most important factors that significantly influence the occurrence of the processes being modeled is important. The absence of such factors in a model can be the cause of incorrect solutions that are adopted on the basis of modeling [5, 13]. In addition, in this case the models are generally unfaithful [14, 15]. It is useful to divide all the factors which can be included in a model of the system under investigation into the following groups [16, 17]:

- essential factors, without whose consideration modeling is impossible;
- principal factors, which play an important role in modeling, but the system does not lose its basic qualities and features in their absence;
- additional factors, whose role in the process or object being modeled is small. They can be called secondary because their variation has practically no influence on the behavior of the system under investigation.

The comparative significance of the factors for any complex process can be evaluated from a quantitative comparison of the criteria obtained by the methods of similarity theory [18, 19].

2.3 Organizing the Work

In this stage of the work, specific approaches to creating a model of the system under investigation are selected on the basis of an analysis of the functional possibilities of different models. The sequence of operations can be described by the following block diagram (Fig. 2.5).

The principal types of material modeling are physical and analog. Both types of material modeling are based on the properties of geometric or physical similarity. For example, two geometric figures are similar if the ratios between all the corresponding lengths and angles are identical. If the similarity factor, i.e., the scale, is known, simple multiplication of the dimensions of one figure by the scale gives the dimensions of another geometric figure that is similar to it. Two phenomena are physically similar if specified characteristics of one can be used to obtain the characteristics of the other by a simple mathematical conversion, which is similar to a conversion from one system of units of measure to another. Similarity theory deals with the study of the conditions for similarity between phenomena. There is

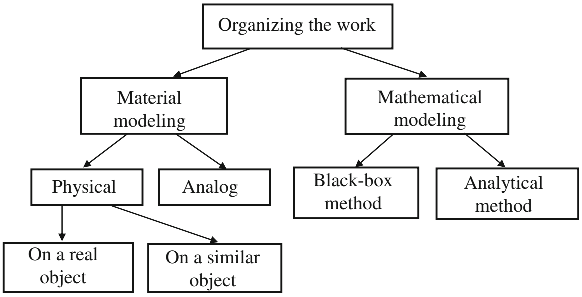

Fig. 2.5 Block diagram of the stage of organizing the work

presently a whole system of dimensionless criteria sets that were obtained by the methods of dimensional analysis [18–20]. They can be used to analyze the features of numerous processes that occur in technological systems. This refers mainly to heat and mass transfer processes. The most important and widely used similarity criteria are listed in Table 2.1.

The possibility of investigating different characteristics on a real object as a whole or on a part of it is also utilized in material modeling and simulation.

The performance of investigations on a real object is called full-scale modeling. The experimental results are also treated using similarity theory. When the object functions in accordance with the stated goal, the laws governing the course of a real process can be revealed. Types of full-scale experiments, such as production and system tests, have a high degree of reliability. A full-scale experiment in the form of material modeling is characterized by the extensive use of automation tools, the employment of diverse information processing tools, and the possibility of human intervention during its performance.

A physical model is a system, apparatus, or device that reproduces a full-scale object on some scale with maintenance of the physical (dynamic) similarity between the processes in the model and in the real system. Physical modeling is a form of modeling, in which an enlarged or reduced material analog is matched to the real object. The analog permits investigation, generally under laboratory conditions, followed by transference of the properties of the processes and phenomena studied from the model to the real object using similarity theory. Physical modeling generally provides a way to obtain reliable results for fairly simple systems.

Analog modeling is based on finding a matching mathematical description for qualitatively different objects [5, 21–24]. Analog modeling is a form of modeling that is based on the similarity of processes and phenomena of different physical nature that can be described in a similar manner by mathematical relations and by logical and structural diagrams (Table 2.2).

Models of the physical and analog types are material reflections of the real object and are closely related to it by their geometric, physical, and strength characteristics. In fact, the process of investigating models of these types reduces

Table 2.1 Principal similarity criteria from dimensional analysis that are used in the investigation of heat and mass transfer processes [18]

Name	Symbol	Formula	Physical meaning
Fourier number	Fo	$\mathrm{Fo} = \frac{at_0}{L_2}$	Ratio between the rate of variation of the conditions in the surrounding medium and the rate of restructuring of the temperature field in a body
Biot number	Bi	$\mathrm{Bi} = \frac{aL}{\lambda}$	Ratio of the temperature drop in a body to the thermal head between the medium and the body
Reynolds number	Re	$\mathrm{Re} = \frac{VL}{v}$	Ratio of the inertial force to the viscous force
Froude number	Fr	$\mathrm{Fr} = \frac{V^2}{gL}$	Ratio of the inertial force to the gravitational force
Euler number	Eu	$\mathrm{Eu} = \frac{\Delta p}{\rho V^2}$	Ratio of the pressure drop to the dynamic head
Péclet number	Pe	$\mathrm{Pe} = \frac{VL}{a}$	Ratio of the convective heat transfer rate to the conductive heat transfer rate
Prandtl number	Pr	$\mathrm{Pr} = \frac{v}{a}$	Ratio of the temperature change in a medium upon passage of a heat flux to the velocity change in the medium upon passage of a momentum flux
Nusselt number	Nu	$\mathrm{Nu} = \frac{\alpha L}{\lambda}$	Ratio of the convective heat transfer rate across a surface to the conductive heat transfer rate across the surface
Mach number	M	$\mathrm{M} = \frac{V}{a}$	Ratio of the flow velocity of a gas to the speed of sound in it.
Bond number	Bo	$\mathrm{Bo} = \frac{\rho g L^2}{\sigma}$	Ratio between the capillary and gravitational forces acting in a system
Weber number	We	$\mathrm{We} = \frac{\sigma}{g(\rho_1 - \rho_2)L^2}$	Measure of the pressure created by interfacial tension forces upon contact between phases
Marangoni number	Ma	$\mathrm{Ma} = \frac{L\Delta\sigma}{\mu a}$	Ratio between the thermocapillary forces and the viscous forces

Note Here L is the characteristic dimension; t is the characteristic time; V is the characteristic velocity; g is the acceleration of gravity; ρ and σ are the density and surface tension of the liquid phase; α, γ, and v are the thermal diffusivity, thermal conductivity, and kinematic viscosity of the material, respectively

Table 2.2 Similarity between fields of different nature in continuous media [1]

Physical process	Process parameter	Coefficient	Relationship between quantities
Heat conduction	Temperature (T)	Thermal conductivity (λ)	Fourier's law (heat flux density) $q = -\lambda$ grad T
Diffusion	Concentration (C)	Diffusion (D)	Fick's law (flux density of matter) $q = -D$ grad C
Direct-current electric field	Potential (U)	Conductivity (G)	Ohm's law (current density) $j = -G$ grad U
Strain (elastic)	Displacement (x)	Elastic modulus (E)	Hooke's law (normal mechanical stress) $\sigma = E$ grad x
Viscous flow of a liquid or gas	Velocity of layers (V)	Dynamic viscosity (μ)	Newton's law (shear stress) $\tau = -\mu$ grad V

to performing a series of full-scale experiments, in which a physical or analog model is used instead of the real object.

From the methodological point of view, two principal approaches to the mathematical modeling of complex systems can be singled out: the black-box method and the analytical method [25–27].

The black-box method is used in cases where the internal structure of the system is unknown or is not of interest to the investigator. The structure of the object of investigation is ignored if its state is characterized only by input parameters, output parameters, and perturbing actions and there is no information about the internal structure of the object. A mathematical model is constructed by establishing a relationship between the input and output parameters through an investigation of the response of the object of investigation to external actions. The methods of experiment planning, as well as variance, regression, and correlation analysis, are widely used for this purpose. The main merits of the black-box method include its simplicity, the highly developed level of its mathematical machinery, and the ensured quality of the modeling result. The shortcomings of this method are associated mainly with the small amount of information that can be derived from the models obtained and the impossibility of evaluating the true causes of the phenomena occurring in the system studied.

Under the analytical approach a model is constructed on the basis of a study of the internal structure of the phenomena occurring in the system. In this case the input and output parameters of the model are related to one another using fundamental physical and physicochemical laws that take into account the internal structure of the modeling object. The mathematical description of the process obtained has a high information content, a broad area of application, and universality. The use of such a model allows understanding the course of the process, and it can easily be combined with optimization procedures. The analytical approach greatly reduces the volume of experiments and improves the efficiency of modeling.

2.4 Developing the Model

This stage is the most critical, because the process studied is simplified specifically here in accordance with the requirements for accuracy, completeness, and information content that are imposed on the models. In the general case there can be several models of a process, which are intended for different goals and which describe the process from different standpoints. The requirements imposed on these models will also be different. The structure of this stage can be represented by the following diagram (Fig. 2.6).

The importance of this stage of the modeling process is confirmed by the need for constant monitoring of its results, which are obtained when each of the procedures presented is performed. This is functionally ensured by iterations during development of the model (Fig. 2.7).

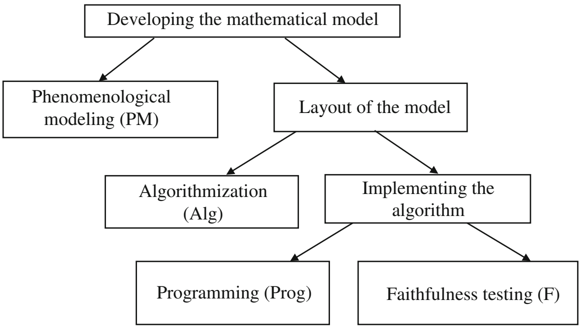

Fig. 2.6 Structural diagram of the stage of developing the mathematical model

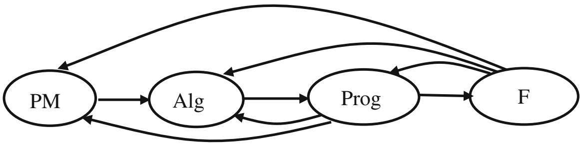

Fig. 2.7 Functional diagram of the stage of developing the mathematical model

We will consider each of the stages singled out on the functional diagram (Fig. 2.7) in detail.

2.4.1 Phenomenological Modeling

Phenomenological modeling is carried out on the basis of the existing information about the modeling object and the requirements placed on the model being created. A phenomenological model usually contains information about the nature and parameters of elementary phenomena in the system under investigation, about the type and extent of the interaction between them, and about the place and significance of each elementary phenomenon in the overall functioning process of the system [28]. Among all the modeling stages, creation of the phenomenological model has been formalized to the smallest extent. However, a highly general approach to the implementation of this stage of the modeling process can be pointed out (Fig. 2.8).

Phenomenological modeling is based on the results of the preceding stages, in which preliminary structuring of the system was performed. When models of real objects and phenomena are constructed, it is generally necessary to deal with a lack of sufficient information. For any object investigated the initial state, the actions, and the distribution of properties associated with them are generally known with some degree of uncertainty. This is due to the limited nature of the number of parameters used in the model, the specific accuracy of the experimental data, and the existence of several factors that are difficult to take into account.

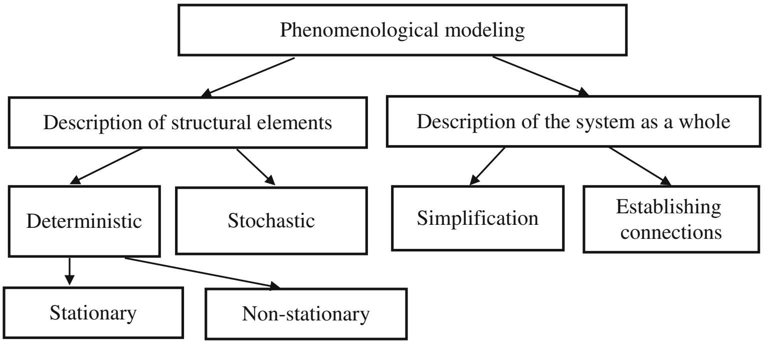

Fig. 2.8 Structural diagram of the phenomenological modeling stage

During construction of a model, the uncertainty of the parameters and individual elements of the structure can be described most simply in the following manner.

- Deterministic—The values of all or certain parameters of the model are specified by deterministic quantities, and a specific integer, a real number or complex number, or an appropriate function corresponds to each parameter. This situation corresponds to complete certainty of the structural units of the system.
- Stochastic—The values of all or certain parameters of the model are set by random quantities, which are assigned by probability densities. Cases of normal (Gaussian) and exponential distributions of the random quantities have been investigated most thoroughly. In certain cases the probability density is determined by treating a restricted experimental sampling of data, which can have an effect on the modeling results.

When the analytical approach is used, the mathematical model generally reduces to a system of differential, integrodifferential, or integral equations of various types. The solution of a given system can uniquely specify the state of the object being modeled and its output parameters at a given time. This uniqueness of the solution also characterizes the deterministic nature of the model. At the same time, random deviations of the state parameters, inputs, and outputs are inherent to any real process. However, these deviations are still insignificant and can be disregarded, and the model itself can be considered deterministic.

The stochastic character of a model is associated with the presence of factors that are not monitored and are simultaneously significant both at the inlet of the system and within it. It is these factors that introduce uncertainty into the modeling results.

The division of parameters into stationary and non-stationary parameters is used for models when one of the independent arguments is time or there is a characteristic that determines the direction of the process or the sequence of its steps.

Stationary models are generally used to describe various flows (liquid, gas, heat) in the case of constancy of the conditions at the flow inlet and outlet. Processes for which the state of the object at each fixed point in space does not vary with the passage of time are called stationary. For such processes time can be eliminated from the list of independent variables. If time or its analog must be employed as one of the significant independent variables of a model, the model is called non-stationary. Such models are usually considerably more complex than stationary models and require large time expenditures for computer realization. In stationary models the input and output parameters, as well as the state parameters of the system, can vary with time, but the functional relationship between them always remains unchanged. The response of a non-stationary system depends both on the current time and on the time of application of the input action. In the case of a shift of the input signal with time without any change in its shape, not only are the output parameters shifted with time, but their shape is also altered. Static models are a special case of stationary models. Their distinguishing feature is the absence of a dependence of all the parameters of the system on the time.

In this stage the level of detail of the phenomenological model at which the model is represented in the form of separate, relatively self-contained subsystems is determined. Naturally, the results obtained during structuring of the modeling object must be taken into account here. The necessary connections between the subsystems identified are revealed. Then each of the subsystems is analyzed separately. Special attention is focused on the conditions for terminating the decomposition of the model. In the general case two such conditions can be singled out.

- The subsystems identified can be described by fundamental laws of physics, chemistry, or other disciplines or by conservation laws.
- Further decomposition is impossible because the necessary data or information is not available.

Thus, in the general case the mathematical model of a system is a multilevel formation consisting of interacting elements that are combined to form the subsystems of the different levels. The result is the creation of a hierarchical sequence of models, each of which reflects the behavior of the system both on a different level of detail and in different physicochemical processes that occur in the system (thermal, hydrodynamic, mass transfer, and other processes). Each subsystem (element) identified has its own characteristic interactions with the other subsystems (elements) and with the external environment [16, 17, 25, 26]. The mathematical model of the system must consist of mathematical models of the separate elements and mathematical models of the interactions between the elements and the external environment. Of course, each element of the mathematical model can have mathematical description with a different level of detail. It is important that the input and output parameters of all the elements of the model would be mutually consistent to ensure that a closed system of equations would be obtained for the mathematical model of the process as a whole. As has already been noted, it is not possible to obtain a description of all the elements and their interactions solely on the basis of fundamental laws. Therefore, for the practical completion of this stage at some level of detail, it is necessary to employ empirical relations and to use definite simplifications. Among the most frequently used methods for simplifying a system, the following can be singled out.

- Stationary (steady-state) processes are analyzed instead of non-stationary processes.
- Random parameters that have a small spread of values are assigned using their mean deterministic values.
- Certain parameters take constant values during the entire modeling process.
- Conditions under which the parameters take specified values are assigned.
- A type of distribution specified by empirical data regarding the behavior of the system under different conditions is assigned for stochastic variables.

Final establishment of the connections between the elements of the system implements the structuring of the phenomenological model of the system under investigation.

In conclusion, we present a recommended sequence of steps for phenomenological modeling:

- analyze the technical and economic reasons behind the statement of the problem;
- establish quantitative criteria for achieving the goal;
- establish and analyze cause-and-effect relationships between the principal physicochemical phenomena and build a structural model of the process;
- analyze the significance of the phenomena;
- define the modeling goal.

2.4.2 Algorithmization

In the case under consideration, algorithmization refers to defining a sequence of mathematical and logical operations that must be performed to obtain a result. This stage of the modeling process can be represented in the form of the following structural diagram (Fig. 2.9).

A diagram is a convenient form for representing the logical structure of models of functioning processes of systems. The logical diagram of a modeling algorithm indicates the time-ordered sequence of logical operations that are associated with the solution of a modeling problem. In the general case three methods for constructing algorithms are distinguished: the verbal, tabular, and graphical (block diagrams and graph diagrams) methods. Generalized and detailed diagrams of modeling algorithms are devised in the various stages of modeling [29, 30].

A generalized (consolidated) diagram of a modeling algorithm specifies the general order of the operations for modeling a system without any refining details. It shows what must be done in each successive step of modeling.

A detailed diagram of a modeling algorithm contains refinements that are lacking in the generalized diagram. A detailed diagram shows what must be done in each successive step of modeling and how it should be done.

The set of symbols defined in ISO 5807:1985 (State Standard 19.701-90) “Information processing—Documentation symbols and conventions for data,

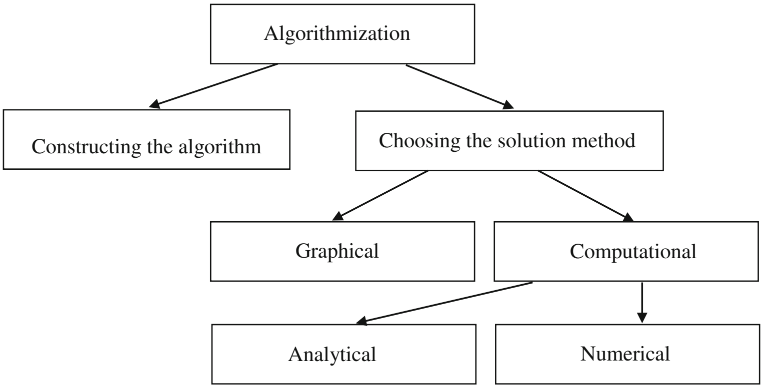

Fig. 2.9 Structural diagram of the algorithmization stage

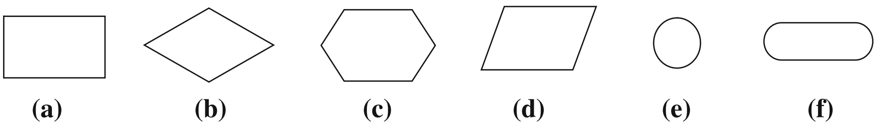

Fig. 2.10 Symbols used in modeling algorithms

program and system flowcharts, program network charts and system resources charts" are used to draw these diagrams. Some of the most commonly used symbols in the practice of modeling are shown in Fig. 2.10.

They include basic (*a*), specific (*b*–*d*), and special (*e* and *f*) symbols:

- *a*—Process—This symbol represents any kind of data processing function.
- *b*—Decision—This symbol represents a decision or a function that has one input and several alternative outputs, only one of which can be activated after calculation of the conditions specified within this symbol.
- *c*—Preparation—This symbol represents modification of a command or a group of commands for the purpose of influencing a certain subsequent function.
- *d*—Manual operation—This symbol represents any process performed by a human.
- *e*—Connector—This symbol represents an exit from one part of the flowchart and entry to another part of the same flowchart and contains the same unique identification.
- *f*—Terminator—This symbol represents an exit to the external environment or an entry from the external environment, or the start or end of the algorithm flowchart.

To use the mathematical models developed, the dependence of certain parameters of the modeling object that were unknown *a priori* and satisfy a certain system of equations must be found. Thus, the search for a solution to a problem reduces to finding certain dependences of the quantities sought on the initial parameters of the model. All the methods for solving the corresponding problems that make up the "core" of mathematical models can be subdivided into graphical, analytical, and numerical methods.

Graphical methods are used least frequently. They give satisfactory results when experimental data are treated and relatively simple equations are solved. Graphical methods can also be used for differentiation and integration.

A method for investigating models is classified as an analytical method if it provides a way to obtain output parameters in the form of analytical expressions, i.e., expressions in which a set of arithmetic operations is used. Algebraic expressions that employ a finite number of arithmetic operations, operations that involve raising a number to an integer power, and root extraction are a special case of analytical expressions. Analytical methods for investigating models are more effective, because they provide a way to study the properties of the modeling object with little computational resources by employing conventional, well developed mathematical methods for the analysis of analytic functions. It is significant that the application of analytical methods is possible without using a computer. In addition, knowledge of analytical expressions for the parameters sought makes it possible to investigate the fundamental properties of the object and its qualitative behavior and to devise new hypotheses regarding its internal structure. It should be noted that the possibilities of analytical methods depend on the level of development of the corresponding branches of mathematics. The currently existing mathematical models provide a way to obtain analytical solutions only for relatively simple mathematical models in a narrow range of parameter values.

In most cases numerical methods, which provide a way to obtain only approximate values of the parameters sought, are used to investigate models. The replacement of real relationships by discrete relationships is common in numerical methods. It is generally achieved by switching from a function of a continuous argument to functions of a discrete argument. The solution of the discrete problem obtained is taken as an approximate solution of the original mathematical problem. When numerical methods are used, a computational algorithm that provides a solution of the discrete problem after a finite number of steps must be developed. Algorithms that require a smaller number of operations to achieve the same accuracy are called *economic* or *efficient*. The *accuracy* of an algorithm refers to the possibility of solving the original problem with an assigned error after a finite number of operations. The magnitude of the error can vary from operation to operation. If the error increases without bound during the calculations, the algorithm is called *unstable* or *divergent*. Otherwise, the algorithm is called *stable* or *convergent*. Three principal components of the resultant error can be distinguished.

- The *unavoidable error* is associated with the inaccurate assignment of the original data of the problem.
- The *method error* is associated with an improper transition to the discrete analog of the original problem.

- The *rounding error* is associated with the finite number of digits in the numbers represented in a computer.

Numerical methods are applicable only to proper mathematical problems. This places a significant restriction on the use of these methods in mathematical modeling. A problem is called proper if it has a unique and stable solution for any values of the original data.

The following numerical methods are used most widely to solve differential equations:

- the finite-difference method (FDM);
- the finite-element method (FEM);
- iterative methods.

2.4.3 Programming

The next stage is the development of computer programs that implement each of the mathematical models of the process on the basis of a program flowchart. A program flowchart represents an interpretation of the logical diagram of a modeling algorithm based on a specific algorithmic language. The program flowchart reflects the logic of the computer implementation of the model using specific modeling software. A set of standard symbols is also used to represent the program flowchart. Before the programming is performed, the program flowchart is verified. For this purpose, each operation represented in the program flowchart and the corresponding operations in the logical diagram of the model are tested. Sometimes control experiments are performed for this purpose. The process of developing reliable and efficient software is no less complicated than the development of the preceding stages in the creation of a mathematical model. Successful resolution of this question is possible only after the modern algorithmic languages, programming technologies, and available software have been thoroughly mastered and knowledge of the technological possibilities and features of the computer implementations of the methods of computational mathematics and experience in solving similar problems have been gained. Modern programming is an independent science with its own fundamental principles, approaches, and methods. Therefore, specialists in this area, i.e., programmers, are enlisted to implement this stage of the work. For this reason, we will dwell only on the general approaches to the implementation of a mathematical model in the form of a computer program.

Most programs that implement mathematical models consist of three parts:

- a preprocessor for preparing and testing of the original data;
- a processor for solving the problem and implementing the computational experiment;
- a postprocessor for displaying the results obtained.

These three component parts can be implemented in the form of a single program only for relatively simple cases. To create modern models of the behavior of liquids, gases, and solids, each of the parts indicated can include an entire set of programs. Preprocessors and postprocessors have special value in modern computer-assisted design (CAD) systems, and they significantly shorten the time needed to retrieve data and evaluate modeling results. A program is more reliable and is created in less time when standard software elements, i.e., packages of applied programs and databases, are used to the maximum extent.

2.4.4 Testing the Faithfulness of a Model

The faithfulness of a mathematical model usually refers to the degree of correspondence of the results obtained using it to the experimental data or a test problem, as well as its ability to satisfy the goals for which it was constructed. Before proceeding to test the faithfulness of a model, convincing evidence of the correct combined functioning of all of its algorithms and programs is needed, i.e., debugging and testing of the programs written are performed. Syntactic, semantic, algorithmic, and other errors in the programs are thereby revealed and eliminated, and the speed and reliability of the computational algorithm chosen are evaluated.

Testing the faithfulness of a model has two goals:

- to ascertain the validity of the collection of hypotheses that were formulated in the preceding stages of the work;
- to ascertain that the accuracy of the results obtained corresponds to the specified accuracy.

The answer to the question regarding the accuracy of modeling depends on the requirements placed on the model and on its purpose. The accuracy of the experimental results or the special features of the statements of the test problems must be taken into account here. For models that are intended for performing estimated calculations, an accuracy of 10–15% is considered satisfactory. For models used in controlling and monitoring systems, the required accuracy must be no less than 1–2%.

The qualitative agreement and quantitative agreement of comparison results are generally distinguished. In a qualitative comparison only the agreement of certain characteristic features in the distribution of the parameters investigated is required. In fact, in a qualitative comparison the agreement of the form of the distribution function of the parameters is evaluated to determine whether it is a decreasing or increasing function, whether it has one or several extrema, etc. A quantitative comparison is made only after there is satisfactory qualitative agreement.

In this stage several aspects of the faithfulness of the model, viz., its consistency, stability, and realism, are tested [6, 27].

The first aspect of faithfulness is the consistency of the model with common sense. First of all, it is necessary to determine the consistency of the model with

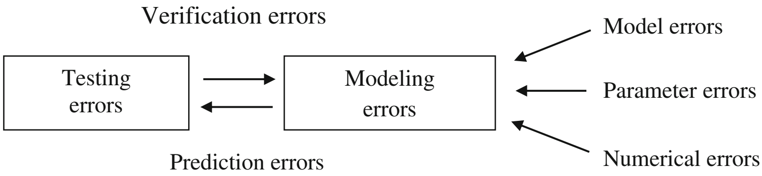

Fig. 2.11 Structure of the errors in the computer simulation and testing of the faithfulness of a model

fundamental physical laws and its compatibility with the action of the most important laws of mechanics and thermodynamics. The model must not contradict the general conceptions regarding the process that were derived from its experimental study. If simulation results confirm the consistency of the model in all the situations indicated, it can be stated that there is a possibility to compare different design solutions using it.

To test for stability (robustness), the sensitivity of the output parameters of the model to small changes in the input parameters within the range of applicability of the model is analyzed. The ability of the model to adjust itself to the influence of these deviations on simulation results is evaluated.

The third aspect of testing for faithfulness is evaluation of the realism of the model, i.e., the correspondence of simulation results with the required accuracy to special cases, for which there are actual data. Testing for realism requires setting up and performing real experiments.

When problems associated with the faithfulness of a model arise, the correction process should begin with a systematic analysis of all possible causes of a disparity between the simulation and experimental results. First, the model should be investigated, and its degree of faithfulness with different values of the variable parameters should be evaluated. If the model is unfaithful in a range of parameters that is interesting to the investigator, an attempt should be made to refine the values of the constants and initial parameters of the model. If this does not produce positive results, the system of hypotheses adopted must be modified. This solution actually means going back to the initial stages of the model development process. Accordingly, it can involve not only profound changes in the mathematical statement of the problem, but also changes in the methods used to solve it, complete revision of the software, and a new faithfulness testing cycle. Therefore, a solution involving modification of the system of hypotheses adopted should be considered from all points of view and adopted only in cases where all other possibilities for improving the faithfulness of the model have been exhausted.

The principal types of errors associated with evaluation of the faithfulness of a model are classified in the following manner (Fig. 2.11) [16, 17]:

- errors in verification of the model using results of control experiments;
- modeling errors associated with the effect of factors that are not taken into account in the model;

- testing errors associated with evaluation of the faithfulness of the model by comparing calculated and experimental data.

The modeling errors have the most complex structure and are subdivided into model errors, parameter errors, and numerical errors.

The end result of all of the stages of the model development process described is a computer model, which can be used to obtain required results from evaluations of characteristics of the process studied (the analysis problem) or to perform a search for the optimal structures, algorithms, and parameters of the system (the synthesis problem).

2.5 Performing a Computational Experiment

The rapid advancement of computer technology has not only helped to speed up various types of calculations, but has also opened new, broader possibilities for the mathematical modeling of complex processes. One of the most important techniques for applying mathematical models in a modern scientific investigation is mathematical (computational) experimentation. It is used both during the preliminary analysis of the systems being modeled (in identifying the parameters of the model and in testing for faithfulness) and during the synthesis of design solutions. A computational experiment is an organized set of investigations, in which devices and processes are studied on the basis of mathematical models using a computer, their behavior under different conditions is simulated, and the optimal parameters and regimes of functioning systems or systems being designed are found. The need to use computational experimentation as a research method is due to the fact that solving modern, extremely complex scientific technical problems by traditional methods has become difficult and, in some cases, impossible.

A computational experiment has many features in common with a real (full-scale) experiment [16, 17].

First, the repeated triggering of the performance of calculations according to a mathematical model on a computer is equivalent to the repetition of trials in a full-scale experiment. The performance of each individual calculation is similar to the performance of a physical experiment: the investigator “switches on” the equations and then follows what happens in the system (as in a real trial).

Second, in a real experiment measurements are performed with some error, and in a computational experiment the solution obtained is generally not exact (especially when numerical methods are used), has a discrete character, and provides only an approximate description of the behavior of the object or process being studied. This is due, in particular, to the fact that many initial parameters of a model are often known only approximately, as are the initial and boundary conditions. All these factors have an effect on the final result of the calculations to a certain extent.

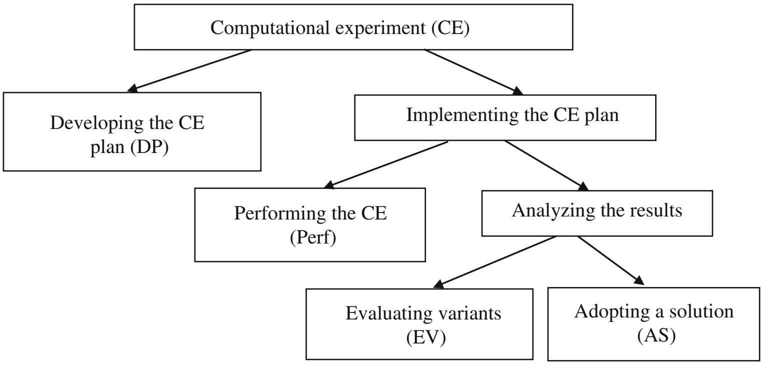

Fig. 2.12 Structural diagram of the computational experiment stage

While a computational experiment has properties in common with a full-scale experiment, it also has some merits and advantages that are inherent only to it. We note the most important among them [16, 17, 27, 31].

- Full-scale experiments often require considerable resources, unique equipment, and the energy and efforts of a large number of specialists. A computational experiment is distinguished by the fact that it is performed on mathematical models of objects, rather than on the objects themselves. The same model can be used to study processes of different physical nature.
- In a full-scale experiment each trial must be set up from the start, while in a computational experiment it is sufficient to modify coefficients of the model and the initial or boundary conditions. Any combination of parameters in the equations of a model can be assigned, even over a fairly broad range.
- A computational experiment can be more easily controlled. This is especially important when the dimensions of the region where the process takes place are small and its duration is short.
- In the case of a dependence of the system being studied on a large number of parameters, consideration of the influence of each of them separately is possible. This is impossible for a full-scale experiment.

The sequence of operations in each stage of the work can be represented in the form of a structural diagram (Fig. 2.12).

It must be noted that the calculation procedure itself should be thought out so that the maximum amount of information would be obtained with the smallest expenditures of resources. In other words, a computational experiment must be planned. The plan specifies the number and order of performance of the calculations on the computer, as well as the techniques for storing and statistically treating the simulation results. The particular problems that can be solved when computational experiments are planned include decreasing the expenditures of machine time on simulations, increasing the accuracy and reliability of the simulation results, testing the faithfulness of the model, etc. Thus, when mathematical modeling is used, it is necessary to rationally plan and design not only the model of the system itself, but also the process in which it is used, i.e., the performance of a computational experiment with it.

Applying the systems approach to the problem of planning computational experiments with models of systems, we can distinguish two planning components: strategic planning and tactical planning [11, 12, 29, 30].

Strategic planning is aimed at solving the problem of obtaining the required information about a system using a model that is implemented on a computer with consideration of the constraints on the resources available to the experimentalist. Strategic planning is essentially similar to the external designing performed when the system is created, except that here the process of modeling the system is the object.

Tactical planning refers to determining the procedure for carrying out each series of tests of the mathematical model that are specified by the experiment plan. For tactical planning there is also an analogy to internal designing of the system, in which the process of working with the model is regarded as the object. The more complex is the mathematical model, the more important is the stage of tactical planning of the computational experiment that is performed immediately before the simulation.

The end result of the computational experiment consists of data expressed in an exact quantitative form from a simulation performed in exact accordance with the plan developed. These data form the basis for the next stage of the work: their comparison with theoretical predictions and data from full-scale experiments. If a significant disparity is observed between the results of the computational experiment and the empirical data, the model is corrected both in the direction of making it more complex and in the direction of simplifying it, and the computational experiment “cycle” is repeated on the improved foundation. This stage of the realization of the computational experiment is continued as long as data that more accurately describe the system under study are obtained as a result of refinements of the mathematical model and the calculation algorithm. The last version of the data can be used to interpret the results and adopt a solution as applies to the modeling goals. Thus, the end result of the computational experiment consists of detailed and specific practical recommendations that are expressed in an exact quantitative form and achieve the specified goal.

Of course, all the procedures in this stage of modeling have an iterative character, which can be expressed in the form of a diagram (Fig. 2.13).

A more general end result of the performance of the computational experiment and analysis of its results is a fully developed mathematical model that is faithful to the assigned conditions and is intended for studying, predicting, and optimizing complex multi-parameter processes.

However, it cannot be assumed that computational experimentation is an ideal method of investigation that has no shortcomings. There are several problems associated with the realization of a computational experiment when complex applied problems are modeled.

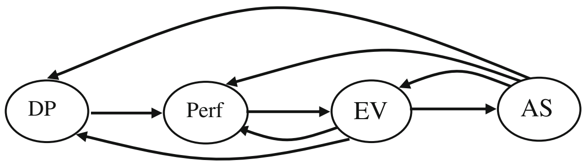

Fig. 2.13 Functional diagram of the computational experiment stage

1. When the number of independent factors included in the mathematical model is large, the investigator may fail to detect fundamental laws and may encounter problems in isolating the main factors that influence the system under study.
2. A computational experiment is limited in the same sense as a full-scale experiment, i.e., it yields discrete information for a certain particular combination of parameters.
3. Since numerical methods are used to solve the system of equations that appear in the mathematical model, a situation in which a loss of stability of the calculations due to a flaw in the algorithm can be interpreted as a loss of stability of the real physical system is possible.
4. It is difficult to evaluate the error due to the replacement of continuous functions by discrete functions and of differential equations by finite-difference expressions. In addition, the possibility of the accumulation of errors due to errors in the rounding of numbers during their processing in the computer must be taken into account.
5. The accuracy of an approximate solution of the problem obtained using classical difference schemes depends on the numerical method chosen, its parameters, and the parameters of the system under investigation.

Therefore, it may be stated that a computational experiment can never replace either a physical experiment or a theoretical analysis of the object or process under study. Only a reasonable combination of all three methods of investigation is a necessary condition for success in solving many problems [32–34].

In conclusion, we present the modeling process in the form of a generalized structural diagram (Fig. 2.14).

2.6 Conclusion

The current trends in the development of high-temperature processes are characterized by the creation of information technologies and their incorporation into scientific research, as well as into technical and technological developments. The technical basis of information technologies is the current, highly efficient computer technology, the methodological basis is systems analysis, and the solution method is mathematical modeling and computational experimentation.

The development of computer hardware and of general and special software gives investigators a powerful tool for solving scientific–technical and engineering problems. The use of "artificial intelligence" enables them to devise and

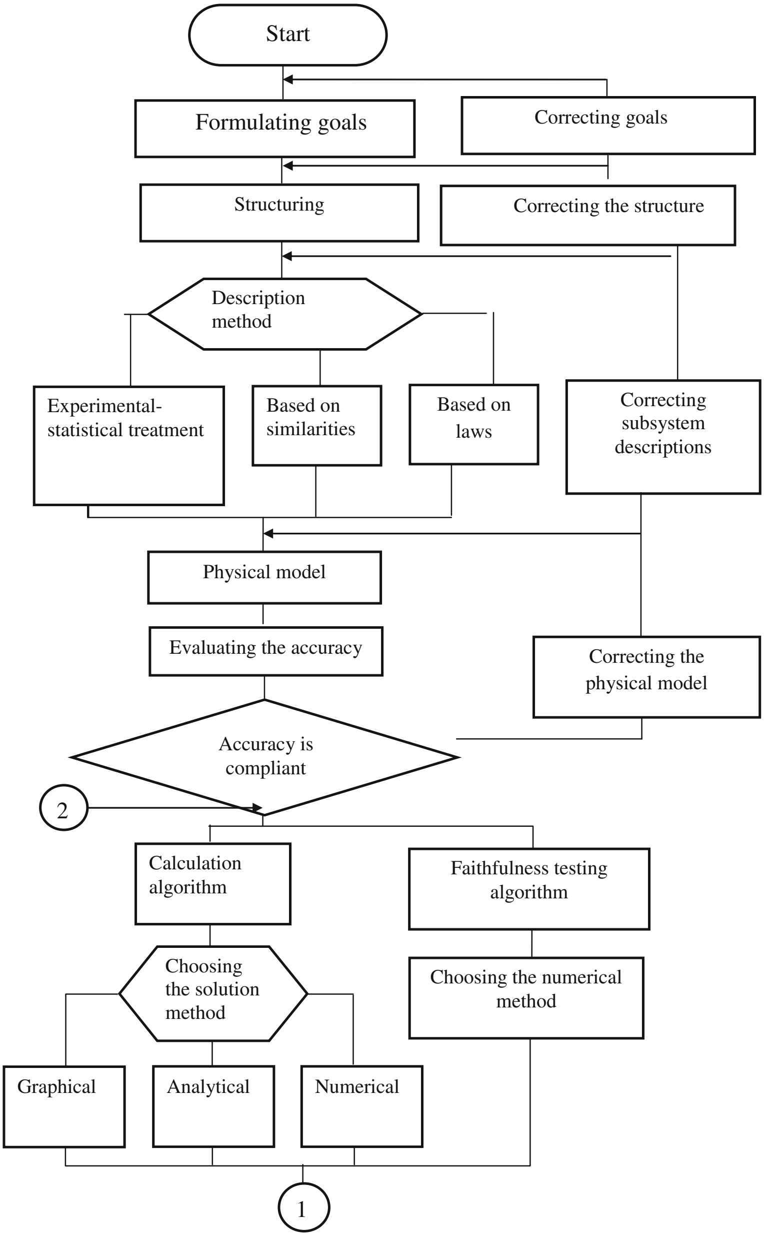

Fig. 2.14 Block diagram of the modeling process

implement complex mathematical models that are simultaneously accurate and meaningful. However, the availability of modern computer equipment and an ability to utilize its continually expanding possibilities are necessary, but not

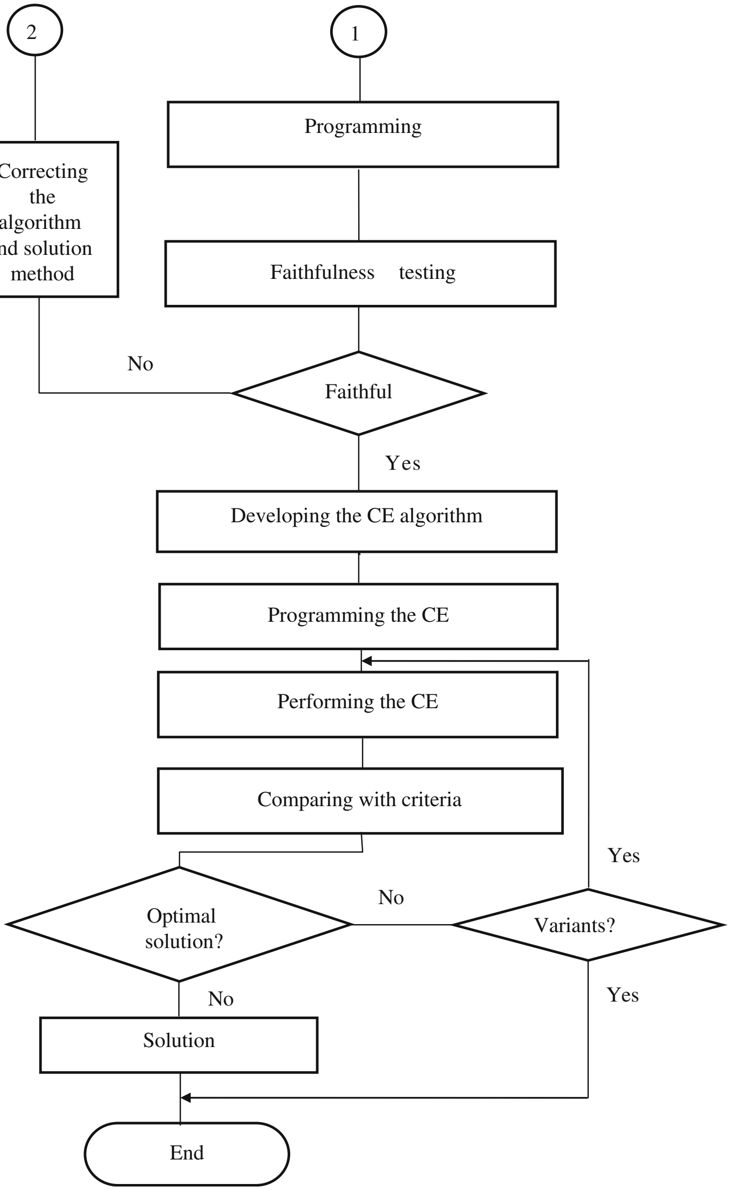

Fig. 2.14 Continued

sufficient conditions for creating effective information technologies. One of the most important conditions for creating faithful mathematical models for complex high-temperature processes is an understanding of the essence of the interactions that occur in multicomponent systems and the laws describing them. Therefore, the investigator's training and professional knowledge in a specific area are fundamental conditions for the development of complete mathematical models that can be used to predict the behavior of objects or the occurrence of processes in them with accuracy that is sufficient for practical purposes.

The theory of systems analysis provides the investigator with a powerful tool for comprehending the surrounding activity by establishing a special type of thinking. Comprehending the essence of an object, process, or phenomenon, the investigator treats it as consisting of a large number of elements, whose interrelationship provides for the integral properties of the entire system. Attention is focused on revealing the variety of connections and relationships that occur both within the object under investigation and in its interrelationships with the external environment. To understand the behavior of the object, process, or phenomenon being modeled and to predict its properties, the investigator must reveal the forms in which matter, energy, and information are transferred from one element to another and ways to control them.

In the current stage the most important conditions for further improvement and intensification of high-temperature technologies include both the development of theoretical foundations for the respective processes using the latest advances in various fields of fundamental and applied sciences and the creation of highly efficient methods and tools for modeling and simulating high-temperature processes, monitoring them, and achieving optimal real-time control.

In the current stage mathematical modeling, whose methods and tools have become the intellectual core of information technologies, is being "incorporated" into the structure of the information community. Modern modeling methods have become a fundamental set of tools for investigating and comprehending processes occurring in complex technological systems.

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