Criteria for Adequacy of Mathematical Descriptions of Physical Processes

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Abstract: - The adequacy criteria for mathematical descriptions in the form of ordinary differential equations are proposed. These descriptions increase the practical value of mathematical simulation results and make it possible to use the results of mathematical simulation to optimize and predict the movement of physical processes. Interrelations between criteria are considered. The proposed criteria are easily transferred to the mathematical descriptions in algebraic form.

Key-Words: - mathematical simulation, adequate descriptions, criteria of adequacy, applications

1 Introduction

Mathematical modelling or simulation is a means of studying the real objects, processes or systems by replacing of the real objects on the mathematical models which are more comfortable to study with the help aid of computers.

The mathematical model is an approximate representation of real-world objects, processes and systems expressed in mathematical terms. In this case significant features of original are saving from researcher's point of view.

The paper presents two criteria for the mathematical description of the physical process which ensure the coincidence of the results of mathematical modeling (using this mathematical description) to experimental data. In addition the fulfillment of these criteria allows using this description to predict the behavior of the physical process and its optimization.

The existing criteria do not provide reliable and stable results of predicting the behavior of the physical process by mathematical methods in a deterministic formulation [1,6].

First of all some definitions and some concepts are given for the convenience of exposition.

A *mathematical model* of a real physical process will be called mathematical dependencies and connections between the elements of a mathematical model. These elements are chosen on the basis of the interests of the researcher himself and the ultimate goals of study of the process. Usually dependencies and relationships have forms of differential equations, integral equations or algebraic connections.

The functions of external influences or external loads, which are present in the mathematical model of the process in the form of symbols, will be called as *models of external loads*.

The initial conditions, boundary conditions and other conditions for the mathematical model will be called as *additional conditions*.

The totality of the mathematical model of the process, models of external loads and additional conditions will be called as *mathematical description* of the process.

The study of the behaviour of the mathematical model of an object under the influence of models of external loads and additional conditions will be called *mathematical modelling or mathematical simulation*.

The practical significance of the results of mathematical simulation of physical processes depends on the degree of coincidence of the results of mathematical simulation of the selected mathematical description of the real process with experimental data [1]. Such property of a mathematical description of a physical process is usually called as *adequacy*.

2 Preliminary Definitions

A mathematical description will be called an *adequate mathematical description* (AMD) of the process under study if the results of mathematical simulation using this description coincide with

experimental data with the accuracy of experimental measurements.

The definition of adequacy will be clarified later for some types of mathematical descriptions.

If the coincidence of the results of mathematical modelling with experiment is bad, then further use of this mathematical description will be problematic.

It is note that authors of works on mathematical modelling concern seldom questions of adequacy of the constructed mathematical description of physical process to real measurements [2-5]. Sometimes such adequacy is proved by the real facts, sometimes authors refer to results of other authors, sometimes there have not any arguments.

The considered situation requires the formation of some uniform approach to this problem, common methodological approach, general algorithms, common criteria of estimation of adequacy degree.

Currently, there are two main approaches to the problem of constructing mathematical descriptions [1,6,7]:

- for a mathematical model with a priori chosen structure and inaccurate parameters, the model of external loads is determined, which, together with the mathematical model of the process, provide the adequacy condition (coincidence with experiment);

- a model of external loads is set a priori, and then parameters of mathematical model and of its structure are selected such way that results of mathematical simulation match up with experiment.

Comparison of the results of mathematical simulation with experimental data in determining an adequate mathematical description ensures the objectivity of the results of the synthesis of a mathematical description. In the literature, the first approach is called the method of identifying external loads [8].

Mathematical models of physical processes can are represented as systems of ordinary differential equations, systems of partial differential equations, algebraic relations, integral equations, etc.

In the given paper the mathematical models of physical processes described by the system of the ordinary differential equations will be examined only [2,3]. Such idealization of real processes or dynamic systems is widely used in various areas for the description of control systems [9], as well as of mechanical systems with the concentrated parameters [5,10], economic processes [11], biological processes [12], ecological processes [13] etc. In some works with the help of such systems human emotions are simulated [14].

Many problems investigated in the given paper have place for other types of mathematical models of physical processes, for example, for mathematical models in the form of the partial differential equations.

The author hopes that the offered criteria of adequacy will be useful in constructing of the adequate mathematical descriptions of real physical processes.

3 Adequacy of Quantitative Type

Consider the adequacy's criteria for mathematical descriptions in the form of differential equations system.

For the simplicity, let us select the physical processes with mathematical models in the form of linear system of ordinary differential equations [15]:

$$\dot{x}(t) = C x(t) + D z(t),$$
 (1)

where *C*, *D* are matrices with constant coefficients which are given approximately, $x = (x_1, x_2, ..., x_n)^T$ – vector-function variables characterized the state of process $((\cdot)^T$ is a mark of transposition), $z(t) = (z_1(t), z_2(t), ..., z_m(t))^T$ is vector-function of external loads; $x \in X, z \in Z, X$; *Z* are normalized functional spaces.

We assume that state variables $x_i(t)$, $1 \le i \le n$ of system (1) correspond to some real characteristics of process $\tilde{x}_i(t)$, $1 \le i \le n$ which are under investigation.

By mathematical description of the physical process we mean the set of the system of equations (1), the vector of the external loads functions $z(t) = (z_1(t), z_2(t), \dots, z_m(t))^T$ and the initial conditions $x(t_0) = x^0$. In other words, a mathematical description is a collection of mathematical model, models of external loads and initial conditions.

The process of solving the system of differential equations (1) under the influence of selected models of external loads $z(t) = (z_1(t), z_2(t), \dots, z_m(t))^T$, taking into account the initial conditions $x(t_0) = x^0$, is usually called *mathematical modelling* or *mathematical simulation*.

An adequate mathematical description of a physical process of the such type with respect to all variables $x_1(t), x_2(t), \ldots, x_n(t)$ of quantitative type will be called the mathematical description for which the results of mathematical simulation of

variables $x_1(t), x_2(t), \dots, x_n(t)$ coincide with the results of experimental measurements $\tilde{x}_1(t), \tilde{x}_2(t), \dots, \tilde{x}_n(t)$ of the characteristic $x_1(t), x_2(t), \dots, x_n(t)$ with the accuracy of the experiment $\delta_1, \delta_2, \dots, \delta_n$:

$$\left\| x_i(t) - \widetilde{x}_i(t) \right\|_X \le \delta_i, \ 1 \le i \le n.$$
 (2)

In practice the measurement of the characteristics of state variables is limited to only one or two components. We formulate a refined definition of the adequacy of a mathematical description for the case of a single variable.

An adequate mathematical description of a physical process of the such type with respect to the variable $x_k(t), 1 \le k \le n$ (ALMD_{xk}) of quantitative type will be called the mathematical description for which the results of mathematical simulation of a variable $x_k(t)$ coincide with the result of experimental measurements $\tilde{x}_k(t)$ of the characteristic $x_k(t)$ with the accuracy of the experiment δ_k :

$$\left\| x_{k}\left(t\right) -\widetilde{x}_{k}\left(t\right) \right\|_{X}\leq\delta_{k}\,. \tag{3}$$

For the rest of the variables, coincidence with experiment is not determined. Adequate mathematical descriptions are similarly determined in the case of several measurements of state variables. The metrics of comparison in this case are determined by the objectives of specific studies.

In the papers [10,16], which were considered before, coincidence with experiment is ten times below the accuracy of experiment.

The criteria of mathematical descriptions adequacy of quantitative type which are offered in the given paper, can be used for other types of mathematical descriptions of physical processes, for example, for mathematical descriptions in the form of the partial differential equations [17]. They have many common features.

It can be shown that there is an infinite set of adequate mathematical descriptions for the same physical experiment.

In addition, qualitatively different physical processes can are have adequate mathematical descriptions for the same experiment. There exist two approaches to problem of construction of adequate mathematical description of quantitative type [6,7,15],:

- 1) Mathematical model of process of type (1) is given a priori with inexact parameters and then the models of external loads were determined for which the results of simulation coincide with experiment [15];
- Some models of external loads are given a priori and then mathematical model of process of type (1) is chosen for which the results of simulation coincide with experiment [6,7].

Now we will consider the synthesis of adequate mathematical description of quantitative type in the frame of first approach analysing the process with the concentrated parameters, for which the motion is described by ordinary linear differential equations of n-order (1).

We assume that some functions of state $x_1(t), x_2(t), \dots x_r(t), r \le n$ in system (1) are obtained from experiment and presented by graphs. Besides, we suppose that some of functions of external loads, for example, $z_1(t), z_2(t), \dots z_l(t), l \le m$ are unknown. According to first approach, it is necessary to construction of such model of external loads under which the results of mathematical modeling of state variables $x_1(t), x_2(t), \dots x_r(t)$ will coincide with experimental measurements $\tilde{x}_1(t), \tilde{x}_2(t), \dots \tilde{x}_r(t)$ with inaccuracy of initial data.

Such mathematical model of process behavior together with obtained model of external loads can be considered as *adequate mathematical description of quantitative type* of process.

This method of obtaining of mathematical models of external loads (functions $z_1(t), z_2(t), \dots z_l(t), l \le m$ is determined in literature as a method of identification [8]. By the way, physical reasons of occurrence of such external loads are not being taken into account. They are only functions which in combination with mathematical model (1) provide results of modelling, which coincide with experiment with the given accuracy.

In work [18,19] were consider the example of a mathematical description that satisfies the criterion of the adequacy of a quantitative type for all variables $x_1(t), x_2(t), \ldots, x_n(t)$. The dynamics of the main mechanical lines of rolling mills was investigated.

For each unknown functions of external loads in system (1) was obtained integral equation Volterra of first kind

$$A_p \ z = u_{\delta} \ , \tag{4}$$

where z is the searched function, u_{δ} is the given element which belong, respectively, to the functional spaces Z and U, A_p is the integral operator.

Since the right-hand side of the integral equation (4) is determined from the experiment, it is natural to assume that instead of the exact right-hand side u_{ex} of the equation (4), some approximation of it is given u_{δ} :

$$\|u_{\delta} - u_T\|_U \le \delta$$
, δ is const. (5)

The set of possible solutions $Q_{\delta} \subset C[0,T]$ of equation (4) consists of elements that correspond to the equation with given accuracy:

$$Q_{\delta} = \{ z : \left\| A_p z - u_{\delta} \right\|_{U} \le \delta \}.$$
(6)

Each function in the set Q_{δ} together with the given mathematical model (1) provides an adequate mathematical description of the physical process.

In this case, the problem of identifying model of external loads in the rolling mill is considered as the inverse problem of the synthesis [15].

In such problems, it does not make sense to consider the question of the accuracy of the obtained solution of the inverse problem, since there is no reasonable function with which it is necessary to compare the obtained solution. In the classical theory of ill-posed problems, the "exact" solution z^{ex} of the integral equation in (4) is taken the function:

$$A_p z^{ex} = u^{ex} \tag{7}$$

However, the function z^{ex} in this case has no practical significance, since the operator A_p is approximately defined, as is the system (1) itself.

By virtue of the properties of the set Q_{δ} in these problems there is the possibility of choosing from Q_{δ} in a certain sense optimal solutions. For example, you can choose from Q_{δ} a variety of solutions with the lowest energy management costs, the solution is the most smooth etc.

The example of astrodynamical processes mathematical description which has property of adequacy of quantitative type in only for one variable was considered in paper [20].

The development of this mathematical model does not take into account important physical factors that have a significant effect on the behaviour of interplanetary matter. To such factors it is necessary to attribute first of all gravitational interaction and heat flows. Because of this, one should not expect a good coincidence of the real characteristics of the physical process with the results of mathematical simulation.

4 Adequacy of Qualitative Type

We will consider what prospects of adequate descriptions are valid for further use and what goals should be selected as the creation of adequate mathematical descriptions.

It will be useful to address to classical works in this area. In work [21] the following statement was done: "...the imitation modelling is the creation of experimental and applied methodology which aimed at the use of it for a prediction of the future behaviour of system ".

So the adequate mathematical descriptions are intended for the forecast of behaviour of real process at first. It is possible with the aid of adequate mathematical modelling to predict behaviour of real process in new conditions of operation. For example, it is possible to test more intensive mode of operations of the real machine without risk of its destruction. Such tool (adequate mathematical description) allows to determine so the optimum parameters of real process.

Let us now consider the conditions under which it is possible to further use adequate mathematical descriptions for ". . . . a prediction of the future behaviour of system".

Obviously, the structure of system (1), its parameters and the specific type of external influences are determined by the properties of a real physical process.

Let the selected structure of the mathematical model of the physical process include parameters $p = (p_1, p_2, ..., p_k)^T$ (for example, the mass of the elements, the stiffness of the elastic elements, etc.), which are reflecting the actual physical characteristics. The structure of the mathematical model also includes dependencies that reflected real physical patterns and dependencies of the process under study.

For the purposes of further substantiated use of mathematical descriptions, it is necessary to require that there is a one-to-one correspondence between the components of the vector parameter p of mathematical description and the actual physical elements. In addition, it is necessary to require that the interconnections between the parameters of a mathematical model comply with the physical laws

of the process being studied and the main external loads had been included. This important correspondence will be called the main correspondence (MC). The execution of the MC will be believed the fulfilment of the criterion of adequacy of the qualitative type. In other words, a mathematical description of a physical process satisfies the criterion of adequacy of a qualitative type if the main correspondence is fulfilled.

An additional requirement for the implementation of the MC is explained firstly by the fact that the quantitative agreement of the results of mathematical modelling with a specific experiment possible for mathematical descriptions of is qualitatively different physical processes due to the selection of parameters of mathematical descriptions.

The implementation of the MC leads to the fact that the models of external influences obtained by the method of identification will correspond to the real external influences on the physical process. At least, these models will not contradict the physical meaning. If we return to the example of the synthesis of an adequate mathematical description of the process of mechanical oscillations in the main line of the rolling mill, then it can be argued that the MC is being executed. By virtue of this, the obtained models of external loads have a reasonable physical interpretation (do not contradict the physical meaning). The external load smoothly increases from zero to a steady-state value.

When fulfilling the adequacy of a mathematical description of a qualitative type, it becomes possible to argue that a mathematical description that satisfies two criteria of adequacy will retain its useful properties for other experiments in the future under small changes in the conditions of the physical process. In other words, this description can be used for "a prediction of the future behaviour of system." An example of such a successful application could be further mathematical simulation using an adequate mathematical description for the rolling mill [19].

In the second example the main correspondence is not fulfilled and, therefore, the application of the obtained results in the new conditions will not be justified.

The algorithm for constructing an adequate mathematical description of a qualitative type cannot be formalized, as in the case of the adequacy of a mathematical description of a quantitative type. The process of constructing such a description mainly depends on subjective factors, such as the scientific problems of studying the physical process using mathematical simulation methods. In some cases, it is impossible to perform a check of mathematical description adequacy of a quantitative type due to lack of experimental data in principle. Let us give an example of a mathematical description that satisfies only the criterion of adequacy of a qualitative type.

An important and relatively new field of applications of methods of mathematical simulation is a tectonic processes study [22]. In this example was used mathematical description for which the criterion of quantitative type can be checked only a posteriori.

Methods of mathematical modelling penetrate recently into many non-traditional areas of human activity such as the study and modelling of emotions [14]. Let us consider in more detail the peculiarities of the application of methods of mathematical modelling in this field.

An obvious difficulty in any model of love is defining what is meant by love and quantifying it in some meaningful way.

In [23] considers a love affair between Romeo and Juliet as the simplest linear model of second order. Note that for this mathematical description the criterion of the adequacy of the quantitative type and the criterion of the adequacy of the qualitative type cannot be check due to the specificity of the process under study. Therefore, the further use of the results of mathematical simulation is unreasonable. However, there are no obstacles to non-traditional interpretations of the results of mathematical simulation of emotional processes.

5 Conclusion

The proposed adequacy criteria for mathematical descriptions in the form of ordinary differential equations make it possible to reasonably use the results of mathematical simulation to optimize and predict the behaviour of physical processes.

These are easily transferred on mathematical descriptions in algebraic form [24].

Criteria for the adequacy of mathematical descriptions in the form of partial differential equations are currently missing in the literature. However, some criteria for the adequacy of mathematical descriptions can be transferred to the specified descriptions.

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