



MATHEMATICAL MODELING OF CHEMICAL-TECHNOLOGICAL PROCESSES, INFORMATION PROCESSING

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Abstract

The article provides scientific and theoretical information on mathematical modeling of chemical-technological processes, data processing.

Keywords: Technological, mathematical, method, expression.

INTRODUCTION

Mathematical modeling is an effective tool for determining optimal control parameters, especially in cases where the laws of physical and chemical processes are sufficiently studied. Based on this, control parameters are determined by calculating the mathematical model of the object in a wide range of external influences. Among the methods of developing mathematical models, the following can be distinguished:

- This analytical method is based on the fundamental laws of substance conservation:
- Experimental and experimental-analytical method is based on the statistical processing of experimental data about the input and output states of the object being studied.

The development of mathematical modeling methods made it possible to change the methodology of researching the technological processes taking place in the apparatus, which is reflected in the discovery of cause-and-effect relationships of events through the hierarchical structures and levels of the entire production and apparatus. The technological process is analyzed from the evaluation of the physical and chemical phenomena occurring in it, to the integral evaluations, taking into account the interactions between individual levels.

An important feature of chemical-technological processes is that the set of phenomena has a deterministic-stochastic nature. Its nature is evident in the compensation of stochastic properties of the hydrodynamic environment to the substance – heat transfer and chemical changes in the apparatus. This is explained by the random interaction of the components of the phases (particle collisions, their crushing, coalescence, random distribution over the volume of the device) or the boundary conditions of the character of the geometry in the device (random arrangement of randomly laid nozzle elements, catalyst grains, the productive orientation of the interphase boundary of moving media, etc.).

Similar systems and components are characterized by extremely complex interaction of their constituents, as a result of which it is impossible to study them from the standpoint of the laws of classical deterministic transport and storage of matter.





How to study chemical-technological processes. Mathematical modeling provides the key to solving this problem. This method is based on a systematic analysis strategy. This is the strategy its essence is to consider the process as a complex interacting hierarchical system, qualitatively analyze its structure, develop its mathematical expression and estimate its unknown parameters. For example, when looking at the events that occur during the movement of an ensemble of particles, droplets or gas bubbles in a homogeneous liquid environment, five levels of the hierarchy of effects are distinguished: 1) a set of events at the atomic-molecular level; 2) effects on the scale of external molecules or globular structures; 3) a set of many physico-chemical phenomena that take into account interphase energy and substance transfer phenomena and chemical reactions, depending on the action of the unit connection of the dispersed phase; 4) physico-chemical processes in an ensemble of mixtures migrating in a single phase; 5) a set of processes that determine the macrohydrodynamic environment at the hardware scale. This approach allows to fully establish the set of events of the entire process and the links between them.

Studying the properties of an object through a mathematical model is understood as mathematical modeling. Its purpose is to determine the optimal parameters of the process, control it based on the mathematical model and transfer the results to the object.

The concept of a mathematical model is the main concept of the mathematical modeling method. A mathematical model is an approximate description of some phenomenon or process of the external world, expressed using mathematical notation.

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Mathematical modeling involves three interconnected stages:

- 1) creating a mathematical description of the studied object;
- 2) choosing a method of solving the system of mathematical description equations and introducing it in the form of a modeling program;
- 3) determining the similarity (adequacy) of the model to the object.

At the stage of creating a mathematical description, the main events and elements of the object are first isolated, and then the relationships between them are determined. For each isolated element and event, an equation (or system of equations) is written that describes its functioning. In addition, equations of connection between various isolated phenomena are included in the mathematical description.

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