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MATHEMATICAL MODELING OF CHEMICAL-TECHNOLOGICAL PROCESSES

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Abstract
The article describes the mathematical modeling of chemical-technological processes and the scientific-methodological processes carried out in this regard.

Keywords: simulation, experimental, invention, mathematical, chemical-technological.

Introduction

Analysis of the cognition methods which have been used since early times reveals that the general methods created in order to investigate life phenomena could be divided into two groups: the application of similitude, modeling and simulation, experimental research which also uses physical models. These methods have always been applied to all branches of human activity all around the world and consequently belong to the universal patrimony of human knowledge. The two short stories told below aim to explain the fundamental characteristics of these cognition methods.

First story. When, by chance, men were confronted by natural fire, its heat may have strongly affected them. As a result of these ancient repeated encounters on cold days, men began to feel the agreeable effect of fire and then wondered how they could proceed to carry this fire into their cold caves where they spent their nights. The precise answer to this question is not known, but it is true that fire has been taken into men's houses, Nevertheless, it is clear that men tried to elaborate a scheme to transport this natural fire from outside into their caves. We therefore realize that during the old times men began to exercise their minds in order to plan a specific action. This cognition process can be considered as one of the oldest examples of the use of modeling research on life. So we can hold in mind that the use of modeling research on life is a method used to analyze a phenomenon based on qualitative and quantitative cognition where only mental exercises are used.

Second Story. The invention of the bow resulted in a new lifestyle because it led to an increase in men's hunting capacity. After using the bow for the first time, men began to wonder how they could make it stronger and more efficient. Such improvements were repeated continually until the effect of these changes began to be analyzed. This example of human progress illustrates a cognition process based on experimentation in which a physical model (the bow) was used. In accordance with the example described above, we can deduce that research based on a physical model results from linking the causes and effects that characterize an investigated phenomenon. With reference to the relationships existing between different investigation methods, we can conclude that, before modifying the physical model used, modeling research has to be carried out. The modeling can then suggest various strategies but a single one has to be chosen.

MAIN PART:

USES OF MATHEMATICAL MODELS:

1. To improve understanding of the process
2. To optimize process design/operating conditions
3. To design a control strategy for the process
4. To train operating personnel

The most important result of developing a mathematical model of a chemical engineering system is the understanding that is gained of what really makes the process "tick." This insight enables you to strip away from the problem the many extraneous "confusion factors" and to get to the core of the system. You can see more clearly the cause-and-effect relationships between the variables.

Mathematical models can be useful in all phases of chemical engineering, from research and development to plant operations, and even in business and economic studies.

Research and development: determining chemical kinetic mechanisms and parameters from laboratory or pilot-plant reaction data; exploring the effects of different operating conditions for optimization and control studies; aiding in scale-up calculations.

Design: exploring the sizing and arrangement of processing equipment for dynamic performance; studying the interactions of various parts of the process, particularly when material recycle or heat integration is used; evaluating alternative process and control structures and strategies; simulating start-up, shutdown, and emergency situations and procedures.

Plant operation: troubleshooting control and processing problems: aiding in start-up and operator training; studying the effects of and the requirements for expansion (bottleneck- removal) projects; optimizing plant operation. It is usually much cheaper, safer, and faster to conduct the kinds of studies listed above on a mathematical model than experimentally on an operating unit. This is not to say that plant tests are not needed. As we will discuss later, they are a vital part of confirming the validity of the model and of verifying important ideas and recommendations that evolve from the model studies.

In this regard, the priority technologies of the Fourth Industrial Revolution, focused on industry and ensuring industrial safety, are technologies related to the processing and identification of patterns in large. volumes of structured and unstructured data and the transition to fully automated digital production.

Controlled by intelligent systems in real time. The basis of these technologies is the use of neural networks in their implementation. Industrial accidents have their own characteristic features, the main ones being the comparative rarity of accidents in comparison with the life cycle of production and a significant range of consequences. The danger of industrial accidents is usually assessed in terms of the possibility of severe damage, or the threat of their causing. Taking into account the tasks and peculiarities of building an industrial safety control system for HIFs, in this article, to assess the risks of emergencies, it is proposed to use an umbrella operational monitoring system to collect parameters that can be used to assess the state of the most critical systems and elements of the controlled object, collect statistics and on its basis calculate the integral indicator of the risk of emergencies. The peculiarity of the implemented approach is that risk assessment is based on analytical processing of information about the prerequisites of accidents and incidents detected at the early stages of the development of dangerous events. This uses reliable, real-time information about the current state of the control object, its components and subsystems . The proposed approach makes it possible to implement proactive management of industrial safety risks,prompt adoption of preventive measures to prevent accidents, pre-accident situations and incidents. When assessing the industrial safety risks of particularly dangerous production facilities, the characteristics of equipment reliability are not always the determining factors. The industrial safety of a complex technological process is influenced by many factors, both external and internal.

The quality of raw materials, weather conditions, impact of automated systems and operating staff on the technological process, professional training of staff and many other factors that can make a decisive contribution to the development of negative phenomena, up to the loss of control over the technological process.

Early detection of these factors is important for timely adoption of preventive measures that will prevent their negative impact.

To study the anomalous behavior of complex technological systems, mathematical modeling methods are usually used, which allow reducing the problem of studying various processes to the problem of studying the properties of a mathematical model, which is a system of equations describing processes.

Methodology

When assessing the characteristics of chemical production, the results of studies of the structure and reactions of substances are verified by experience with subsequent recommendations for practical use. Modeling the properties and reactivity of chemical compounds makes it possible to predict the course of chemical processes.

The further construction of a mathematical model of the chemical process will be considered using the example of styrene production, the initial data for which were obtained experimentally. Styrene is a raw material for the production of polymers and copolymers (polystyrene, synthetic rubber). The reactions of obtaining styrene proceed at a temperature of the order of 600-700 degrees. If the production technology is violated, styrene may be released into the environment, which may be accompanied by an explosion. The aim of the article is to build a mathematical model of the styrene production process in order to predict its behavior under changing input conditions. The main idea of the analysis of a complex dynamic model of behavior is that the basic structure of the behavior of such a system, which contains information about the system, namely the attractor of the dynamic system (that is, a subset of the phase space that attracts trajectories in the limit of infinite time), can be reconstructed through the measurement one observable characteristic of this dynamic system, fixed as a time series.

Forecasting a time series is expressed in the approximation of a function of many variables for a given set of examples using the procedure of immersing the series in an m-dimensional lagged space. For a sufficiently large m, it is possible to guarantee an unambiguous dependence of the future value of the series. on its m previous values, i.e. forecasting a time series is not reduced to an approximation, but to the interpolation of a function of many variables. A neural network is used to restore this unknown function from a set of examples given by the history of a given time series.

The ideas underlying the theory of artificial neural networks are based on a number of theorems, according to which any multidimensional continuous function can be represented as sums and products of one-dimensional functions. Therefore, with the help of correctly designed neural networks, it is possible to make predictions in situations that are extremely complex from the point of view of nonlinear dynamics.

The main idea of nonlinear dynamics is that fewer variables may be required to describe a system than the general case. Then the system can be characterized by its low-dimensional projection.

It is proposed to use a mathematical model of (ANN) to link input parameters and output characteristics. ANN is an effective method for simulating processes that allows identifying complex relations between input and output characteristics.

The mathematical modeling process includes the following stages: 1.data preparation; 2. neural network formation;

1. Neural network testing. First stage: data preparation. At the first stage, data analysis was performed, and the dependences of the parameters of the styrene production on time, pressure and temperature were considered. For the transition to the common units, it is necessary to carry out their normalization:

2. Neural network training: = 2(x-x)-1,Xmax-Xmin x→[-1;1]. Normalization is performed when data of different dimensions is fed to different inputs of neurons. If there is no normalization, the values at the second input will always have a significantly greater impact on the network output than the values at the first input. When normalizing, the dimensions of all input and output data are brought together.

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