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SYSTEMS ANALYSIS OF CHEMICAL-ENGINEERING PROCESSES*

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Using systems analysis one can successfully solve problems in mathematical simulation, optimization, and optimal design of chemical-engineering systems at the workshop, factory, and combine level. However, the principles of systems analysis, with its powerful formal mathematical apparatus, has not so far been widely used at the level of the individual chemical-engineering process. Nevertheless, a single chemico-technological process with all its complex of individual physicochemical effects is a complex system. Its level, which is characterized by a variety of elementary physicochemical effects, saturation of the mutual relations between them, and the compatibility and interaction between phenomena of different physicochemical kinds in a local volume of space, is so high that it is among the most complex cybernetic systems.

The book under review describes the fundamental aspects of a new systems approach to the analysis, design, and simulation of the processes occurring in chemical engineering.

The first chapter is devoted to a qualitative analysis of a complex physicochemical system, two aspects of which can be distinguished: the semantic and the mathematical. Here an effective apparatus is used for the semantic analysis of the structure of a complex process comprising the construction of a diagram showing the mutual influences of the elementary physicochemical effects in the system. Then the structure of the mathematical relations which are the foundation of the description of physicochemical systems is analyzed. Two common approaches are analyzed: the phenomenological and the statistical.

On the basis of the phenomenological approach the structure of the fundamental relations describing the motion of a multiphase, multicomponent, continuous medium, which can serve as the initial basis for solving many mathematical problems relating to physicochemical systems, is investigated. In particular, starting from the module of interpenetrating continua, the equations of the mechanics of a multicomponent two-phase compressed disperse mixture, in which heat- and mass-transfer processes occur together with chemical reactions, are formulated. The energy transfers which occur in heat and mass transfer between phases are analyzed. The particular features of the mechanics of two-phase multicomponent mixtures related to the nonideal nature of the phases are explained. The problems involved in taking into account the nonequilibrium characteristics of multicomponent mixtures in the equations of motion of such media are considered. Starting from the assumption that the internal energy of the mixture is additive with respect to the masses of the phases and the assumption of local equilibrium within a phase, the individual problems of thermodynamics of heterogeneous multicomponent media are analyzed: An explicit expression is obtained for the dissipative function of the system, an analysis is made of linear phenomenological relations, and the particular features of the structure of direct and cross effects which develop in the system are analyzed. A closed system of thermohydrodynamic equations of a two-phase multicomponent disperse medium is obtained, representing the mass, force, and energy interactions between the phases.

It is shown, using the other approach, that the statistical Gibbs ensemble method can serve as the fundamental mathematical simulation of the stochastic features of many physicochemical systems characteristic of chemical engineering. The balance equation of the properties of the ensemble for seeking the multidimensional distribution function of the particles with respect to the physicochemical properties is formulated as the mathematical model of the processes occurring in polydisperse media, and examples of its application are given.

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In the following three chapters, possible approaches to the synthesis of functional operators of physicochemical systems are described: formal methods of setting up a mathematic idea of a "black box" (Chap. 2); methods of setting up a mathematical description of a complex system on the basis of general models of the mechanics of continuous media (Chap. 3); methods of describing processes in chemical engineering using typical models of hydrodynamic structures of flows in technological apparatus (Chap. 4). The material is systematically organized and is accompanied by a large number of well-chosen examples which illustrate the particular features of this new methodical approach to the solution of important problems in the chemical, petrochemical, and microbiological industry. Methods of constructing models of mass-transfer, chemical, heat, and microbiological processes in polydisperse media are described in particular detail using examples.

The last four chapters are devoted to modern methods of checking the adequacy of mathematical descriptions of complex physicochemical systems and the identification and estimate of the parameters of the state of chemicotechnological processes. It is shown that the central problem at this stage of the simulation is the computational difficulty due to the incorrectly posed nature of the problems in the classical sense. Methods of overcoming these difficulties are described. The monograph is written at a high scientific level, uses a systematic approach, and is essentially practical. It gives for the first time a detailed description of the fundamentals of systems analysis as they apply to chemical-engineering processes. The book provides the fundamentals of the modern theory of chemical-engineering processes.

The authors are well known as leading specialists in the field of cybernetics of chemical-engineering processes and systems analysis. Its main aspects are original developments by the authors in this area. The material in the book is methodically set out, the latest achievements of Soviet and world science in this field are widely used, and modern mathematical methods are employed (the methods of mathematical physics, the mathematical theory of dynamic systems, the mathematical theory of optimality, the theory of mass servicing, the theory of graphs, the theory of inverse problems in mathematical physics, etc.).

A large class of systems considered in the book are nonlinear physicochemical systems distributed in space and time. In our opinion, it would have been more complete to give those sections which touch on the identification and estimation of the parameters of nonlinear and distributive systems. The same comment applies to the topological principle of the simulation of physicochemical systems: The method of constructing process-construction diagrams is merely recalled. We hope that in other monographs by the authors or in a reprint these problems will be given the necessary consideration.

On the whole, the book is important and timely. It is the first work published in the USSR in which, using a new methodological approach, modern methods of analyzing and designing chemical-engineering processes are considered in a systematic manner. It should be of considerable use to scientists working in the area of theoretical chemical technology, control theory, and the optimization of chemical-engineering processes, physicochemical hydromechanics, and theoretical and applied cybernetics.