SYSTEMS ANALYSIS OF HEAT AND MASS TRANSFER

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Methodological principles of systems analysis of the processes of heat and mass transfer are presented. The concept of a complex physicochemical system is introduced and principles of a strategy for analyzing heat-exchange processes and synthesizing their mathematical description are formulated.

Scientific—technical progress in all sectors of the national economy (including the chemical, petrochemical, and petroleum refining industries) depends to a large degree on the efficient use of scientific resources, the quality and results of scientific investigation, and a high level of development of the theoretical principles of production-process technology.

An important factor in improving the quality of scientific investigation is its organization into the form of a comprehensive scientific treatment, consisting of the study of the given object using the methods of various sciences, the elaboration of an integral theoretical picture of the phenomenon in question, and, on this basis, the development of specific scientific recommendations for practical applications.

The logical—mathematical foundation of such a comprehensive treatment is systems analysis, which combines several scientific disciplines — cybernetics, information theory, the general theory of complex systems, semiotics, etc. At all levels of the chemical industry, the systems approach has become the primary approach used in solving problems of design, optimization, management, and optimum planning.

At the level of individual production operations, however, the principles of systems analysis and the powerful formal apparatus of the latter have not yet been sufficiently widely used. Together with this, an individual production process — with its complex set of component physicochemical phenomena — is a typical large system. The variety of the attendant phenomena, the degree to which these phenomena are interrelated, and the combination and interaction of phenomena of a different physicochemical nature within a local volume of the production unit are of such a magnitude as to make the individual chemical production process one of the most complicated cybernetic systems.

The prerequisites for a systems approach to analyzing and designing chemical production processes were supplied by works dealing with the theoretical foundations of chemical technology, continuum mechanics, the thermodynamics of irreversible processes, chemical thermodynamics, and mathematical methods of investigating complex systems.

Despite the obvious advances made thus far in the quantitative description of chemical production processes, abetted by the development of methods of physical and mathematical modeling and the broad use of computer technology, the construction of an adequate description of production processes is often impeded by the lack of a comprehensive approach to the problem based on the strategy of systems analysis. This is particularly true of processes with a complex internal structure. Foremost among such processes are hydrodynamic, diffusive, and thermal processes occurring in inhomogeneous polydispersed media and complicated by the simultaneous occurrence of a large number of effects of a different physicochemical nature. Here, a comprehensive solution to the problem is that which, on the basis of the use of methods of different sciences — phenomenological mechanics of inhomogeneous media, theory of heat and mass transfer, statistical hydromechanics, thermodynamics of irreversible processes, chemical thermodyanmics, and the general theory of complex systems — offers an integral theoretical picture of the process in question and, on this basis, permits specific recommendations to be made to solve practical problems.

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The processes of heat and mass transfer are usually analyzed from deterministic positions, it being assumed here that they can be described according to phase by equations of heat and mass transfer, using for each phase the classical deterministic equations of Fourier and Fick for thermal and diffusive flows.

For engineering calculations, these equations are usually reduced to dimensionless criterional equations of the familiar form $Nu = APe^m Pr^n$ and, using the principles of physical similitude, the constants A, m, and n are determined empirically. Within the empirical limits of change in the determining parameters, equations such as the above make it possible to sufficiently accurately design heat- and mass-transfer equipment for single-phase steady flows with a fixed solid surface (wall). However, in the case of the multiphase, multicomponent systems most characteristic of heat-exchange processes, the above approach proves to be wholly inadequate because it does not take into account the stochastic nature of the effects.

The stochastically determined nature of the effects of heat and mass transfer and their nonsteady character under conditions of a constantly renewed phase boundary, polydispersion, fragmentation, and coalesence — distorting the effect of the hydrodynamic and thermal fields on the distribution of concentrations at both micro- and macrolevels — make it necessary to examine the process of heat and mass transfer as a complex, dynamic, stochastically determined physicochemical system.

Formalizing the process of heat and mass transfer, we introduce the concept of a physicochemical system (PCS), in which the process of heat and mass exchange is taking place. In the general case, the PCS is a multiphase, multicomponent continuous medium distributed in space and variable over time. Transfers of matter, energy, and momentum occur at each point of homogeneity of the PCS and at the phase boundaries in the presence of sources (sinks) of matter, energy, and momentum.

From the point of view of the above definition, the process of heat and mass exchange may be represented as a set of stochastically determined effects occurring in a PCS characterized by a high degree of complexity and definable in terms of its hierarchical structure and the quantity of information contained within it.

Systems analysis of the processes of heat and mass exchange includes three stages: qualitative analysis of the structure of the PCS; mathematical description of the PCS or synthesis of its functional operator (mathematical model); determination of the adequacy of and identification of the mathematical model of the PCS [1, 2].

Qualitative Analysis of the PCS

Within the framework of the qualitative analysis of the PCS, a priori information on the physicochemical features of the object are formalized in the form of diagrams illustrating the mutual effects of the physicochemical phenomena in which the nodes correspond to individual phenomena and the oriented arcs correspond to assumed cause-and-effect relations between them [1]. The many physicochemical phenomena characteristic of a PCS are broken down into levels (degrees) and a hierarchy of levels within the general structure of PCS phenomena is established. Apart from the clarity of illustration offered by representing the structure of the PCS at different levels of detail, this technique permits direct quantitative analysis using the mathematical tool of inexact sets, formulations, and algorithms in order to obtain preliminary quantitative information on the system [3].

Five levels may be distinguished in the hierarchical structure of the PCS with regard to the heat and mass transfer phenomena being discussed [1]:

1) the set of phenomena on the atomic-molecular level; 2) effects on the scale of supermolecular or globular structures; 3) the set of physicochemical effects associated with the movement of a single inclusion of a dispersed phase, as well as phenomena of interphase energy and mass transfer; 4) physicochemical processes in an ensemble of inclusions moving in constrained fashion in a layer of continuous phase; 5) the aggregate of processes determining the macrodynamic conditions on the scale of the equipment.

1. The first level of the hierarchy of PSC effects is characterized by physicochemical interactions on the molecular level. The system is considered homogeneous, i.e., the particles (molecules) are ideally mixed, and the character of development and occurrence of the physicochemical processes is determined exclusively by the physical properties of the

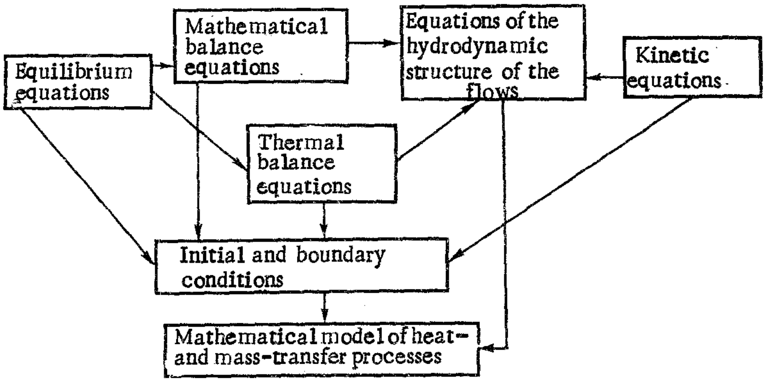

Fig. 1. Overall structure of mathematical model of mass transfer processes.

above particles and the molecular viscosity, thermal conductivity, and coefficients of molecular diffusion. Environmental effects are important among the external factors which affect the physicochemical interactions between the particles. These phenomena manifest themselves in the form of kinetic, diffusive, thermodynamic, and topological changes in the medium.

2. The second level of the PCS hierarchy is the set of physicochemical effects on the level of molecular globules. The structure of a chemically uniform system (i.e., a system of the first level) is complicated from a hydrodynamic point of view by the formation of supermolecular structures or globules within it. By such globules, we mean aggregates of closely situated molecules that exhibit relative thermodynamic stability (integrity) under the influence of hydrodynamic perturbations. Each globule behaves as an "elementary" physicomechanical system exhibiting the entire range of thermal and diffusive effects. The system, completely broken down into individual aggregates of molecules, is evenly distributed throughout the volume of the apparatus and is referred to as completely segregated. The phenomenon of segregation is characteristic of both continuous and dispersed phases. Segregation, and its effects on transfer processes, are particularly manifest in systems with a high viscosity.

The above-examined aggregate of phenomena of the first and second levels is a component part of the effects of higher degrees of the PCS hierarchical structure.

3. The following phenomena may be classed as belonging to the third level in the PCS hierarchy. An element of the dispersed phase (bubble, droplet) in which mass exchange is occurring both within the volume and at the phase boundary is moving in the continuous phase under the influence of buoyancy forces, inertial forces, and drag, being subjected at the same time to the effect of the mechanism of mass, energy, and momentum transfer through the phase boundary. It is natural to assume that nonequilibrium of the heterogeneous system is the initial reason for the appearance of the interphase flows of substances responsible for the entire aggregate of effects comprising the mechanism of interphase transfer. This nonequilibrium may be divided into several types: nonequilibrium with respect to temperature, composition, and velocity, i.e., a difference in the velocity of the phases. Each type of nonequilibrium first of all causes the transfer of the corresponding substance, at the same time having a cross (indirect) effect on the transfer of the other substances.

The flows of mass and energy cause a change in the enthalpy of the continuous and dispersed phases, and also account for other physical and thermodynamic characteristics of the phases: viscosity, density, heat capacity, composition, temperature, etc. The changes in the physicochemical characteristics of the phases, in turn, affect the degree to which the heterogeneous system deviates from equilibrium.

The transfer of mass and energy across the phase boundary also determines local irregularities in the surface tension of the boundary. These local changes in surface tension, in turn, are the main reason for the appearance of spontaneous interphase convection. This convection may be divided into two types: ordered, and disordered. The latter affects mass transfer between the phases as well as leading to deformation of the phase boundary, i.e., to a change in its shape and curvature.

The flow of momentum through the phase boundary at each point of the surface is the vector sum of two components: normal and tangential to the boundary. These components are responsible for the generation of circulation currents within inclusions. These currents intensify the processes of mass and heat transfer in elements of the dispersed phase. The normal and shear stresses at the phase boundary reorient the inclusion in space, changing the trajectory of its motion, and deform the phase boundary.

Differences in the dynamic head of the turbulent eddies at individual points of the phase boundary contribute substantially to deformation of the boundary. The deformation may be so great that the boundary ruptures and the inclusion is broken up into smaller elements. The breakup of inclusions can occur only under the influence of eddies that are of relatively low magnitude. The probability of severe deformations and inclusion fragmentation is diminished in the presence of large-scale eddies that are invariant over distances of the order of an inclusion diameter.

Velocity nonequilibrium of the phases leads to the appearance of surface diffusion, as a result of which surfactant is "blown to the stern" of the moving inclusions, thereby resulting in a nonuniform distribution of the surfactant over the surface of the inclusions. This effect contributes significantly to the nonuniformity of the surface tension of the phase boundary and results in the appearance of additional drag (in competition with the shear stresses) which extinguishes the circulation currents inside the inclusions.

Several effects are associated with deformation of the phase boundary, the most important of which are the following: a) fragmentation of droplets or bubbles and, connected with this, a change in the area of the phase boundary; b) the development of interphase turbulence from spontaneous emulsification and appearance of the phenomenon of surface elasticity; c) a change in the thermodynamic characteristics within the volume of the inclusion: saturation pressure, temperature, composition, degree of deviation from equilibrium, etc. The above-noted effects, connected with deformation of the phase boundary, intensify the processes of the interphase transfer of mass, energy, and momentum.

4. The following effects belong to the fourth level of the PCS hierarchical structure. Each element of the dispersed phase, with the constrained motion of the inclusions in the limited volume of the continuous medium, leaves behind it a turbulent wake. Under the influence of mainly Zhukovskii forces, the eddies from the individual wakes interact with one another and produce turbulence throughout the continuous phase. The surface of the inclusions located in the zone of interaction of the turbulent wakes are enveloped by the eddies of the continuous phase and brought into turbulent motion. This affects the whole aggregate of physicochemical effects of the third hierarchical level. In particular, the change in the trajectory of movement of the inclusions raises the possibility of their collision and coalesence and, thus, a redistribution of the fields of concentration, temperature, and pressure within elements of the dispersed phase. At the same time, the turbulent pulsations of the continuous medium are damped as a result of dissociation of their energy into heat, which in turn causes a change in the heat content of the continuous phase.

With the movement of a single inclusion in an unlimited volume of continuous medium, corresponding tensor fields of concentration, temperature, velocity, pressure, and other physicochemical characteristics are induced in the volume. In an actual production unit (apparatus), the continuous phase is limited in volume by the dimensions of the apparatus, and the movement of elements of the dispersed phase is of a mass nature. This leads to deformation of the concentration, temperature, and velocity fields. The above-described aggregate of effects is an essentially complex process, which we will refer to as the constraint effect.

Phenomena associated with the fourth level of the PCS hierarchy determine the hydrodynamic conditions in a local volume of the apparatus, and the term "local hydrodynamics" is naturally used for the characteristics in this case. The local hydrodynamics are manifest within a certain volume (which is considered elementary, due to its small dimensions in relation to the dimensions of the apparatus as a whole), although the dimensions of this volume are such that an isolated element in the volume contains sufficiently many dispersed-phase inclusions. The main quantitative characteristics of the PCS at this level of the hierarchy are the normal and shear stresses, strain and strain rate, viscosity and diffusion coefficients, thermal conductivity, phase transformation rates, etc.

Usually, the semiempirical concept of locality is based on a determination of the ratio of the coefficient of turbulent exchange to the kinematic viscosity. The specifics of a given theory of interphase transfer depend on the specific methods used to divide the integration interval and determine the coefficient of turbulent exchange at the phase boundary.

The above-examined effects associated with the first, second, third, and fourth levels of the hierarchical structure of the PCS are closely related to one another and form the set of so-called microhydrodynamic factors, affecting the process of the transfer of substances in a heterophase multicomponent system.

5. The fifth level of the PCS hierarchical structure is the aggregate of phenomena which determine the hydrodynamic conditions on the macrolevel in the apparatus. This set of effects characterizes the hydrodynamic structure of the flows in the unit as a whole (rather than in an individual local volume of the unit).

The initial factor determining the specifics of the fifth-level effects is the design features of the apparatus itself. Such features include the dimensions of the unit, the types of mixing and heat-exchange equipment, the location of inlet and outlet nozzles, the presence and shape of baffles, diffusers, trays, distributing devices, etc. The following depend directly on these and other design features of the unit: the supply of external mechanical energy to the unit to provide for mechanical mixing within the system; the exchange (supply or withdrawal) of thermal energy, connected with the design features of the heat exchangers and the mode of delivery of the heat carriers; hydrodynamic, concentration, and thermal perturbations introduced with the incoming flows of the initial reactants.

The combined effect of three factors — mechanical mixing, perturbations introduced with the incoming flows, and the geometric features of the working volume of the apparatus — lead to the formation of a certain topology of the flows. This topology, i.e., the hydrodynamic structure of the flows in the unit, is defined the character and location (within the space of the working volume of the unit) of macrohydrodynamic irregularities: stagnant zones, by-passes, zones of laminar and turbulent flow, circulation currents, etc.

In the process of changes in the hydrodynamic structure of the flows in the apparatus, its basic quantitative characteristics change as well: the distribution of particles of the continuous and dispersed phases with respect to trajectory and time in the unit (which limits the capacity of the unit in terms of each phase), the distribution of the dispersed-phase inclusions with respect to size, etc. The features of the hydrodynamic structure of the flows and the geometry of the apparatus affect the formation of concentration and temperature fields within the volume of the apparatus. The perturbations from the incoming flows and the mode of delivery of thermal energy to the unit also contribute importantly here.

Each level of the above-examined hierarchical structure of the PCS is characterized by a corresponding form of mathematical description. The basis for the description of the first level is comprised of the phenomenological and statistical methods of physicochemical kinetics and chemical thermodynamics. The central problem at this level is interpreting the mechanisms of molecular interactions and calculating kinetic constants — the coefficients of molecular diffusion.

At the second level of the hierarchy, the information of the preceding level is augmented by and interpreted with allowance for data on the degree of segregation of the system and the structure of the supermolecular formations. The tools at this level are mathematical models of segregation of the flows, as well as various theories of heterophase processes.

Description of effects of the third level is based on methods of the mechanics of small-scale flows around dispersed-phase inclusions and of the thermodynamics of surface effects, methods of investigating the equilibrium of multicomponent systems, and various theories of interphase transfer.

The effects of the fourth level of the PCS hierarchical structure may be described using the methods of the statistical theory of continua, methods of the mechanics of dispersed systems, models constructed on the basis of mathematical methods of the kinetic theory of gases, etc.

Equations of the first, second, third, and fourth levels of the hierarchical structure of the physicochemical system constitute a component part of the mathematical description of phenomena of the fifth level, being a mathematical description of subsystems of the entire system on the scale on the apparatus. Experience shows that this description should, first of all, be sufficiently simple and convenient. Thus, the information from the lower levels should be compressed as much as possible and arranged in a sufficiently simple and compact form for use at the fifth level. The information is compressed by evaluating the quantities entering into the description of the lower levels in terms of relative magnitude (order of smallness); finding the most significant factors affecting the production process, using relatively simple models with simplified mathematical descriptions instead of exact relations, etc.

Description of Mathematical Model of Heat- and Mass-Exchange Processes

It is apparent from an analysis of the hierarchical structure of PCS phenomena that a characteristic feature of the system in question is its dual stochastically determined nature. Among the important stochastic features of this system are the character of distribution of elements of the phases with respect to time in the unit; the form of distribution of dispersed-phase inclusions with respect to size; the effects of mechanical interaction of the phases, leading to the collision, breakup, and coalescence (agglomeration) of inclusions, the character of distribution of inclusions with respect to degree of chemical change, viscosity, density, and other physicochemical properties.

An effective procedure for analyzing the above-examined effects from a single point of view is offered by the methods of phase space and statistical emsembles [4]. Each individual inclusion of the dispersed phase is characterized by a position in space, a velocity, and a certain set of state parameters. By analogy with the μ-space of a statistical ensemble of elementary particles in statistical physics, we introduce a multidimensional phase space of a polydispersed PCS, the coordinates $\mathbf{x}$ of which are divided into two groups: external — coordinates of the position and velocity of the k-th inclusion $\mathbf{x}_k^{(e)} = (x_{1k}^{(e)}, \ldots, x_{6k}^{(e)}$; internal — state parameters $\mathbf{x}^{(i)} = (x_{1k}^{(i)}, \ldots, x_{\xi k}^{(i)})$. Each element of the dispersed medium is represented by its own point in the phase space, so that the entire dispersed phase is characterized by the set of these points, forming the so-called "phase gas." Let us introduce phase-gas particle probability density $p(\mathbf{x}, t)$, defining the probable number of representative points in an element of the volume $d\mathbf{x} = d\mathbf{x}^{(e)} d\mathbf{x}^{(i)}$ about the point $\mathbf{x}(\mathbf{x}^{(e)}, \mathbf{x}^{(i)})$, as $p(\mathbf{x}, t)d\mathbf{x}$. The following normalizing condition must be met

$$\int p(\mathbf{x}, t)\partial\mathbf{x} = 1.$$

The balance equation for the number of representative points has the form

$$\frac{\partial p(\mathbf{x}, t)}{\partial t} + \sum_{i=1}^{6} \frac{\partial}{\partial x_i^{(e)}} [v_i(\mathbf{x}, t)\, p(\mathbf{x}, t)] + \sum_{j=1}^{\xi} \frac{\partial}{\partial x_j^{(i)}} [v_j(\mathbf{x}, t)\, p(\mathbf{x}, t)] = q(p(\mathbf{x}, t), t), \tag{1}$$

where $v_i(\mathbf{x}, t)$ is the i-th component of the velocity of the representative points in the phase space; $q(p(\mathbf{x}, t), t)$, a term characterizing the rate of generation or destruction at moment t of particles with the coordinates $\mathbf{x}^{(e)}$, $\mathbf{x}^{(i)}$ due to their interaction and the presence of external sources and sinks; ξ, number of internal generalized coordinates of the system.

Taking as internal coordinates such physicochemical characteristics of the dispersed-phase inclusions as the residence time of the particles in the apparatus τ, the characteristic dimension or volume of the particles r, the concentration of the k-th key component in the particle c_k, temperature T, density ρ, and viscosity μ, we write Eq. (1) in expanded form

$$\frac{\partial p(\mathbf{x}^{(e)}, \mathbf{x}^{(i)} t)}{\partial t} + \sum_i \frac{\partial}{\partial x_i^{(e)}} [v_i(\mathbf{x}^{(e)}, t) p(\mathbf{x}^{(e)}, \mathbf{x}^{(i)}, t)] + \frac{\partial}{\partial \tau}\left[\frac{d\tau}{dt} p(\mathbf{x}^{(e)}, \mathbf{x}^{(i)}, t)\right] + \frac{\partial}{\partial r}\left[\frac{dr}{dt} p(\mathbf{x}^{(e)}, \mathbf{x}^{(i)}, t)\right] + \sum_{k=1}^{n} \frac{\partial}{\partial c_k} [I_k p(\mathbf{x}^{(e)}, \mathbf{x}^{(i)}, t)] + \frac{\partial}{\partial T}\left[p(\mathbf{x}^{(e)}, \mathbf{x}^{(i)}, t)\right.$$

$$\times \sum_{j=1}^{N} \frac{\Delta H_j}{c_p} I_j \Bigg] + \frac{\partial}{\partial \rho}\left[\frac{d\rho}{dt} p(\mathbf{x}^{(c)}, \mathbf{x}^{(i)}, t\right] + \frac{\partial}{\partial \mu}\left[\frac{d\mu}{dt} p(\mathbf{x}^{(e)}, \mathbf{x}^{(i)}, t)\right] = q(p(\mathbf{x}^{(e)}, \mathbf{x}^{(i)}, t), t), \qquad (2)$$

where $\mathbf{x}^{(i)} = (\tau, r, c_1, \ldots, c_n, T, \rho, \mu)$; $I_k = dc_k/dt$, rate of the chemical reaction in the dispersed phase with respect to the k-th key component; n, number of key components out of the total number of components reacting in the dispersed phase; ΔH_j, calorific value of the j-th reaction; N, number of reactions in the dispersed phase; c_p, heat capacity of the dispersed phase.

The balance equation for the properties of the particle ensemble (2) (BPE equation) is valid for any dispersed system that can be described by continuous functions of state, so that it is sufficiently universal in nature. It always serves as the basis of that part of the mathematical model of the PCS which describes the stochastic properties of polydispersed PCS's. The BPE equation is an effective means of studying the stochastic properties of many heat- and mass-exchange processes in polydispersed media — the processes of mass crystallization, extraction, absorption, redistillation, etc. The BPE equation is closely allied with the practically important concept of the distribution of elements of a flow over the residence time in an apparatus. It is apparent from the structure of the BPE equation that the DRT (distribution of flow residence time) function is one of the cross sections of multidimensional density of the distribution function $p(\mathbf{x}^{(e)}, \mathbf{x}^{(i)}, t)$ in the BPE equation with respect to the internal coordinate τ — time of residence of the particles in the apparatus. This explains the fact that the main mathematical models of the hydrodynamic structure of flows in apparatus based on the DRT concept are a direct outgrowth of the BPE equation (1).

The description of the determined component of the functional operator of the PCS is based on phenomelogical equations of the thermohydrodynamics of multiphase multicomponent systems in which chemical reactions occur jointly with heat- and mass-transfer phenomena. Generalized closed systems of equations of thermohydrodynamics have been formulated on the basis of representations of mutually penetrating multivelocity continua for two cases: 1) a monodispersed mixture of two phases where there is multicomponent mass and heat transfer with chemical changes; 2) a polydispersed medium with phase transformations, with a random particle size distribution. For the first case, assuming the symmetry of the stress tensor for the continuous phase and the absence of the effect of electromagnetic fields, the following system of equations of thermohydrodynamics was obtained [5]:

$$\frac{d_1\rho_{1k}}{dt} + \rho_{1k}\nabla\mathbf{v}_1 = -\nabla\mathbf{j}_{1k} + J_{k(21)} - J_{k(12)} + \sum_{r=1}^{N} \nu_{k(1r)} I_{(1r)} \quad (k = 1, 2, \ldots, n);$$

$$\frac{d_2\rho_{2k}}{dt} + \rho_{2k}\nabla\mathbf{v}_2 = -\nabla\mathbf{j}_{2k} + J_{k(12)} - J_{k(21)} + \sum_{r=1}^{N} \nu_{k(2)} I_{(2r)} \quad (k = 1, 2, \ldots, n);$$

$$\frac{d_1\rho_1}{dt} + \rho_1\nabla\mathbf{v}_1 = J_{(21)} - J_{(12)};$$

$$\frac{d_2\rho_2}{dt} + \rho_2\nabla\mathbf{v}_2 = J_{(12)} - J_{(21)}; \quad \frac{\partial a}{\partial t} + \nabla(a\mathbf{v}_2) = 0;$$

$$\rho_2\frac{d_2\mathbf{v}_2}{dt} = -\alpha_2\nabla P + \mathbf{f}_{(12)} + J_{(12)}(\mathbf{v}_{(12)} - \mathbf{v}_2) - J_{(21)}(\mathbf{v}_{(21)} - \mathbf{v}_2) + \sum_{k=1}^{n} \rho_{2k}\mathbf{F}_{2k};$$

$$\rho_1\frac{d_1\mathbf{v}_1}{dt} = -\alpha_1\nabla P + \nabla^q\boldsymbol{\tau}_1{}^q - \mathbf{f}_{(12)} + J_{(21)}(\mathbf{v}_{(21)} - \mathbf{v}_1) - J_{(12)}(\mathbf{v}_{(12)} - \mathbf{v}_1) + \sum_{k=1}^{n} \rho_{1k}\mathbf{F}_{1k};$$

$$\rho_1\frac{d_1u_1}{dt} = \frac{\alpha_1 P}{\rho_1^0}\frac{d_1\rho_1^0}{dt} + \varkappa_1\mathbf{f}_{(12)}(\mathbf{v}_1 - \mathbf{v}_2) + \tau_1^{ql} e_1^{qi} +$$

$$+ J_{(21)}\frac{(\mathbf{v}_{(21)} - \mathbf{v}_1)^2}{2} - J_{(12)}\frac{(\mathbf{v}_{(12)} - \mathbf{v}_1)^2}{2} - \sum_{k=1}^{n} J_{k(21)}(i_1 - i_{1k,s}) -$$

$$-\sum_{k=1}^{n} J_{k(12)}(i_{2k,s} - i_1) + q_{(21)} - \nabla q_1 + \rho_1 Q_1 + \sum_{k=1}^{n} \mathbf{F}_{1k}\mathbf{j}_{1k};$$

$$\rho_2\frac{d_2u_2}{dt} = \frac{\alpha_2 P}{\rho_2^0}\frac{d^2\rho_2^0}{dt} + \varkappa_2\mathbf{f}_{(12)}(\mathbf{v}_1 - \mathbf{v}_2) + J_{(12)}\frac{(\mathbf{v}_{(12)} - \mathbf{v}_2)^3}{2} -$$

$$
-J_{(21)}\frac{(\mathbf{v}_{(21)}-\mathbf{v}_2)^2}{2}-\sum_{k=1}^{n}J_{k(21)}(i_{1k,s}-i_2)-\sum_{k=1}^{n}J_{k(12)}(i_{2k,s}-i_2)
$$

$$
-q_{(21)}-\nabla\mathbf{q}_2-\rho_2Q_2+\sum_{k=1}^{n}\mathbf{F}_{2k}\mathbf{j}_{2k}\ ;
$$

$$
P_1=P_2=P;\ \ \alpha_1+\alpha_2=1;\ \ \alpha_2=c_jad_2^3;\ \varkappa_1+\varkappa_2=1;\ \rho_1^0=\rho_1/\alpha_1\ ;
$$

$$
\rho_2^0=\rho_2/\alpha_2;\ \sum_{k=1}^{n}\rho_{1k}=\rho_1;\ \sum_{k=1}^{n}\rho_{2k}=\rho_2;\ \mathbf{j}_{1k}=\rho_{1k}(\mathbf{v}_{1k}-\mathbf{v}_2)\ ;
$$

$$
\mathbf{j}_{2k}=\rho_{2k}(\mathbf{v}_{2k}-\mathbf{v}_2);\ \frac{d_l}{dt}\equiv\frac{\partial}{\partial t}+\mathbf{v}_1\nabla\equiv\frac{\partial}{\partial t}+v_l^q\frac{\partial}{\partial x^q}\ (q,\ l=1,\ 2,\ 3). \tag{3}
$$

Here, the first and second equations are the equations of the weight content of the k-th component in the continuous phase (phase 1) and the dispersed phase (phase 2); the third and fourth equations are the equations of the weight contents of phases 1 and 2; the fifth equation is the balance equation for the number of particles; the sixth and seventh equations are the equations of motion of phases 1 and 2; the eighth and ninth equations are the equations of the flow of heat to phases 1 and 2.

For the second case, the system of integrodifferential thermohydrodynamic equations, including the particle-size distribution function f(r) as the unknown variable, has the form [6]:

$$
\frac{\partial\rho_1}{\partial t}+\nabla(\rho_1\mathbf{v}_1)=-\int_0^R\rho_2^0f\eta dr\ ;
$$

$$
\rho_1\frac{dc}{dt}=-\nabla\mathbf{j}+(c-m)\int_0^R\rho_2^0f\eta dr\ ;
$$

$$
\frac{\partial f}{\partial t}+\nabla(f\mathbf{v}_2)+\frac{\partial}{\partial r}(f\eta)=q_{\text{tru}}\ ;
$$

$$
\rho_1\frac{d_1\mathbf{v}_1}{dt}=-\alpha_1\nabla P+\nabla^q\boldsymbol{\tau}_1^q-\int_0^R\rho_2^0fr\mathbf{f}_{(12)}dr+\rho_1\mathbf{F}_1-\int_0^R\rho_2^0f\eta(\mathbf{v}_2-\mathbf{v}_1)dr;
$$

$$
\frac{D_2\mathbf{v}_2}{Dt}=-\frac{\nabla P}{\rho_2^0}+\mathbf{f}_{(12)}(r)+\mathbf{F}_2(r)\ ;
$$

$$
\rho_1\frac{d_1u_1}{dt}=\tau_1^{ql}\ e_1^{ql}+\int_0^R\rho_2^0fr\mathbf{f}_{(12)}(\mathbf{v}_1-\mathbf{v}_2)dr+\rho_1Q_1+\int_0^R\rho_2^0f\eta\frac{(\mathbf{v}_2-\mathbf{v}_1)^2}{2}dr-\int_0^Rq_{1\sigma}dr-\Delta\mathbf{q}_1\ ;
$$

$$
(\rho_2^0fr)\frac{D_2u_2}{Dt}=-q_{2\sigma}(r)-\nabla\mathbf{q}_2(r)+(\rho_2^0fr)Q_2(r)\ ;
$$

$$
f\frac{D_2u_\sigma^1}{Dt}=q_{1\sigma}+q_{2\sigma}-\rho_2^0f\eta(i_2-i_1)\ ;
$$

$$
\mathbf{q}_i=-\lambda_i\nabla T_i;\ q_{i\sigma}=4\pi d^2f\beta_i(T_i-T_\sigma)\ (i=1,\ 2);
$$

$$
\alpha_1+\int_0^R rf(r)dr=1;\ \ \rho_1=\rho_2^0\alpha_1;\ \rho_2^0=\text{const};\ \mathbf{j}=\rho_1c(\mathbf{v}_{1k}-\mathbf{v}_1)\ ;
$$

$$
\frac{d_1}{dt}\equiv\frac{\partial}{\partial t}+v_1^q\nabla^q;\ \ \frac{D_2}{Dt}\equiv\frac{\partial}{\partial t}+v_2^q\nabla^q+\eta\frac{\partial}{\partial r}\ . \tag{4}
$$

Here the first and second equation describe the weight contents for the carrier phase and the solution; the third equation is the balance equation for the number of particles; the fourth and fifth equations are the equations of motion of the carrier and fourth phase, respectively (the r-th phase is taken to mean a group of particles of volume r); the sixth, seventh, and eighth equations describe the flow of heat to the carrier phase (r-th phase) and phase boundary, respectively.

The notation used in systems of equations (3) and (4) is explained at the end of the article. Systems (3) and (4) play an important role in the overall strategy of systems analysis of the processes of heat and mass transfer, since they serve as the starting point for the transition to simpler descriptions in the solution of specific problems.

One of the most important trends in the synthesis of a functional operator for a heat- and mass-transfer process occurring in a production unit is the transition to simplified (idealized) representations of the internal structure of the physicochemical processes taking place in the system. This approach is based on a set of typical structures (standard models of processes in chemical engineering). Each of the standard idealized models reflects a given type of transfer or transformation of a substance and is characterized by an appropriate functional operator. The block principle [7, 8] is used in constructing the complete mathematical model. According to this principle, after a set of elementary processes has been established, each process is examined separately (in blocks) under conditions that approximate the actual service conditions of the object of the modeling as closely as possible. As a result, each elementary process operator is made to correspond with an elementary functional operator with parameters that are sufficiently close to the actual values.

Representation of the mathematical model of the process in the form of an ensemble of subsystems (blocks) in turn makes it possible to represent the procedure of its construction as a set of operations formulating the mathematical models of the individual subsystems, i.e., it makes it possible to realize the block principle. The overall structure of the mathematical model of mass transfer processes is shown in Fig. 1.

The use of the block principle of constructing mathematical models of the processes in question, based on the systems approach, also helps indicate ways to solve such important practical problems as scaling diffusion processes. From the position of mathematical modeling, the change in scale amounts to nothing more than determining the mathematical model with a change in the geometric dimensions characterizing the equipment formulation of the process. When the block principle of constructing a mathematical model is employed, the effect of the geometric dimensions on the properties of the process is manifest only in one subsystem, namely the "Hydrodynamics" subsystem. Thus, the change in scale can be made, given a mathematical description of this subsystem that is sufficiently accurate in both the quantitative and qualitative senses.

In principle, each block of the mathematical model may have a different degree of detail of mathematical description. It is necessary only that the input and output variables of all of the blocks of the model be mutually consistent, so as to obtain a closed system of equations for the mathematical model of the process as a whole. As concerns the composition of the internal variables of the blocks, there is a fairly large freedom of choice. Ideally, the mathematical description of each block would include equations whose parameters are only physicochemical properties of the separable components of the mixture, as well as geometric characteristics of the equipment and factors accounting for assigned external effects. However, at present, it is not always possible to obtain such detailed descriptions of the individual blocks. This is generally connected with the excessive complexity of the mathematical description of the block, which in turn seriously complicates the mathematical model of the process as a whole and, moreover, may lead to certain computational difficulties. Thus, in the practical application of the block principle, it is sometimes necessary to employ empirical relations to mathematically describe each block at a given level of detail.

The main problem in calculating the quantity of a substance transferred between phases is determining the rate of this transfer. It is well known that there are several models of such a transfer: two-film model; boundary diffusion layer model; surface permeation and rejuvenation model; adsorption model; interphase turbulence model. All of these models in one way or another explain the character of mass transfer between phases, but none of them — except for the interphase turbulence model — account for the interaction of the flows of the phases during their movement, even though the counterflow motion most characteristic of industrial processes has a significant effect on the hydrodynamic conditions on free surfaces.

The most general form of mass-transfer equations allowing for the interaction of phase flows may be obtained using the principle of systems analysis and the qualitative descriptions of the third, fourth, and fifth degrees of hierarchical interaction in a PCS offered above.

Given a nonsteady two-phase flow, due to the variable velocities of the phase flows and the variable physicochemical characteristics following from the conditions of interphase turbulence [8], with the introduction of the factor of the hydrodynamic state of the two-phase system

$$f^* = \left(\frac{L}{G}\right)^a \left(\frac{\rho_g}{\rho_l}\right)^b \left(\frac{\mu_i}{\mu_g}\right)^c,$$

where L, G are the liquid and gas flows; ρ_i and ρ_g, their respective densities; μ_i and μ_g, viscosities, the equations of mass transfer in the stochastically determined interpretation take the form:

for the gas phase

$$\mathrm{Nu}_{dg} = A\,\mathrm{Re}_g^m \mathrm{Pr}_g^n (1 + f^*) \tag{5}$$

for the liquid phase

$$\mathrm{Nu}_{di} = A\,\mathrm{Re}_i^m \mathrm{Pr}_i^n\,(1 + f^*)\,. \tag{6}$$

With $f^* = 0$, Eqs. (5) and (6) are converted to the mass-transfer equations obtained from the two-film model and, for all practical purposes, describe mass transfer in a single-phase flow or a flow with a fixed solid boundary.

In accordance with the structure of mass-transfer equations (5) and (6), the quantity of transferred substance is determined by the transfer of the substance into the phase in which the transfer takes place most slowly, i.e., where most of the drag is concentrated. Thus, if the gas is readily soluble in the liquid, then Eq. (5) is used. If it is not readily soluble in the liquid, then Eq. (6) is used. Accordingly, the mass-transfer coefficients in the Nusselt numbers are divided by the coefficients of molecular diffusion of that phase in thich the process takes place most slowly. The Prandtl number of the phase where most of the drag is concentrated is introduced in exactly the same way, but since the coefficient of molecular diffusion appears in the denominator on both sides of the equations, the resulting effect of this coefficient on the mass-transfer coefficient will depend on the index in the Prandtl number; the higher this index, the less the effect of molecular diffusion on the mass-transfer coefficient.

Since the Prandtl number characterizes the ratio of velocity and concentration profiles, which are determined by the molecular characteristics, we can expect the effect of this ratio on process of mass transfer to change in relation to the hydrodynamic conditions, i.e., there should be a change in the index in the Prandtl number. With the most uniform distribution of the liquid and gas in a two-phase flow under conditions of developed free turbulence, in accordance with the structure of Eqs. (5) and (6), the index n should reach a maximum value equal to unity. With a reduction in the turbulence of the flows, the index n of the Prandtl number should decrease, reaching a limit of zero when movement ceases. In the latter case, the concept of a ratio of velocity and concentration profiles loses its meaning. In practice, in accordance with normal hydrodynamic behavior modes of diffusion flows, the index n of the Prandtl number should change within the limits from 1/3 (laminar mode, if we may conditionally apply this terminology to a two-phase flow) to 1 (mode of developed free turbulence). Specially designed experiments have shown this to be the case [9].

Permitting an analogy to be made between friction and mass exchange in a single-phase gas flow, we may determine the order of magnitude of the exponents m and n in Eqs. (5). Energy consumption on friction in a single-phase flow is determined by the shear stress, which is proportional to the pressure drop:

$$\Delta P_g = -\rho_g(\nu + \varepsilon_p)\frac{dv^q}{dx^l}\ (q \neq l), \tag{7}$$

where ρ_g is the density of the gas; ν and ε_p, coefficients of molecular and eddy viscosity. Accordingly, the diffusion flow is described as follows:

$$q = -(D_m + D_t)\,\frac{dc}{dx}\,. \tag{8}$$

Taking into account the order of magnitude, the last two relations may be represented as follows:

$$\Delta P_g = -\rho_g (\nu + \varepsilon_p) v/l, \tag{9}$$

$$q = -(D_m + D_t)\,\Delta c/l. \tag{10}$$

Having divided (10) by (9), assuming that the mass and energy transfer take place over the same length l, and solving relative to $q/\Delta c$, we obtain

$$\frac{q}{\Delta c} = \frac{(D_m + D_t)\,\Delta P_g}{\rho(\nu + \varepsilon_p)\, v}. \tag{11}$$

But since $q/\Delta c = K$ (K is the total mass-transfer coefficient), Eq. (11) may be represented in the form

$$K = (D_m + D_g)\,\Delta P_g/\rho_g(\nu + \varepsilon_p)\, v. \tag{12}$$

Given the same value of the dynamic-state factor f^* for the two-phase system, the coefficients of turbulent transfer of mass D_t and energy ε_p are of the same order of magnitude. Thus, the following proportional relationship is established between the coefficient of mass-transfer K, the pressure drop ΔP_g, and the flow rate v:

$$K \sim \Delta P_g/v. \tag{13}$$

Equation (13) allows us to evaluate the order of magnitude of the exponents in Eq. (5) for different hydrodynamic conditions.

Three types of dependences of the pressure drop ΔP_g on flow rate v are possible: for a laminar mode, $\Delta P_g \sim v$; for a turbulent mode, $\Delta P_g \sim v^{1.8}$; for developed turbulence (progressive mode), $\Delta P_g \sim v^2$. We can evaluate the exponents in the generalized mass-transfer equation (5) with numbers Re_g and Pr_g. For the laminar mode, $\Delta P_g \sim v$, so that $K \sim v^0$. However, since $\mathrm{Re}_g = vd_e/\nu$, $m = 0$, $n = 1/3$. Thus, for the laminar mode we obtain the following mass-transfer equation

$$\frac{Kd_e}{D_m} = A_0\left(\frac{v}{D_m}\right)^{1/3}(1 + f_0), \tag{14}$$

from which for the laminar made

$$K \sim D_m^{2/3}. \tag{15}$$

Since factor f_0^* is very small (less than unity) under conditions of very low flow rates, Eq. (14) reduces to the form

$$\mathrm{Nu}_d \simeq \mathrm{const.} \tag{16}$$

Equation (16) expresses the condition of molecular transfer of the substance, being a special case of the more general equation (5).

For the turbulent mode, $\Delta P_g \sim v^{1.8}$, so that $K \sim v^{0.8}$: $m = 0.8$; $n = 2/3$, and the mass-transfer equation assumes the form

$$\frac{Kd_e}{D_m} = A_1\left(\frac{vd_e}{\nu}\right)^{0,8}\left(\frac{\nu}{D_m}\right)^{2/3}(1 + f_1^*). \tag{17}$$

It follows from Eq. (17) that

$$K \sim D_m^{1/3}. \tag{18}$$

For the mode of developed free turbulence, $\Delta P_g \sim v^2$, so that $K \sim v$; $m = 1$; $n = 1$, and the mass-transfer equation takes the form

$$\frac{Kd_e}{D_m} = A_2\left(\frac{vd_e}{\nu}\right)\left(\frac{\nu}{D_m}\right)(1 + f_2^*). \tag{19}$$

It follows from Eq. (19) that

$$K \sim D_m^0, \tag{20}$$

i.e., mass transfer under conditions of developed free turbulence is practically independent of molecular diffusion and viscosity. By eliminating the molecular characteristics on on the left and right sides of Eq. (19), the latter can be written as follows:

$$K = A_2 v (1 + f_2^*) \tag{21}$$

or in dimensionless form

$$\frac{K}{v} = A_2 \left[1 + \beta_2 \left(\frac{L}{G} \right)^{a_2} \left(\frac{\rho_g}{\rho_i} \right)^{b_2} \left(\frac{\mu_i}{\mu_g} \right)^{c_2} \right]. \tag{22}$$

Since, under conditions of developed free turbulence, the factor may significantly greater than unity, Eq. (22) is written thus:

$$\frac{K}{v} = A_3 \left(\frac{L}{G} \right)^{a_2} \left(\frac{\rho_g}{\rho_i} \right)^{b_2} \left(\frac{\mu_i}{\mu_g} \right)^{c_2}, \tag{23}$$

and the coefficients of molecular diffusion are omitted from the equations; exponent c_2 is small, close to zero.

The hydrodynamic-state factor of the two-phase system may be independently determined. Meanwhile, it follows from an analysis of the hydrodynamics of the two-phase flow that factor f^* will be a function of a dimensionless complex number which expresses the relationship between the principal variables in the following degrees:

$$f^* = \psi \left[\left(\frac{L}{G} \right)^{2-m} \left(\frac{\rho_g}{\rho_i} \right) \left(\frac{\mu_i}{\mu_g} \right)^{m} \right].$$

Analysis of the mechanism of mass transfer in a single-phase flow shows that the analogy between friction and heat and mass exchange is valid only at numbers $\mathrm{Pr}_d = 1$, i.e., for gases. For liquid droplets, for which Pr_d is of the order of 10^3, the analogy does not hold. Thus, the indices for the numbers Re_i and Pr_i cannot be predicted, and their values in Eq. (6) have to be determined empirically.

Determination of Adequacy and Identification of the PCS Mathematical Model

The final step in the systems analysis of mass-exchange processes is checking the adequacy and identifying the operators of the PCS (of the mathematical models). For systems described by linear differential equations, in checking for adequacy the parameters of the model are found by analyzing the empirically determined DRT function. This analysis is usually done by the moments method. To represent the behavior of the PCS in the general (nonlinear) case, it is sometimes sufficient to perform a linearization and to study the behavior of the system in the vicinity of the assigned steady-state mode.

We can also use the principle of discrete (independent) determination of parameters of the model such as the coefficients of resistance, heat transfer, or mass transfer using physical modeling. It should be noted that the structure of the functional operator of the PCS usually consists of two parts: a linear part, reflecting the hydrodynamic structure of the flows in the production unit, and a nonlinear part, reflecting the kinetics of the physicochemical changes.

Of course, a search for the parameters of the PCS operator should be attempted within the class of linear operators using the methods for identifying linear systems. However, this is possible only in those cases where the degree of nonlinearity of the system in question is sufficiently slight and the errors of the determination fall within tolerable limits. If the degree of nonlinearity is substantial, it is generally not possible to remain limited to a linear description of the object, and the problem of identification must be solved within the class of nonlinear operators.

A promising approach to evaluating the functional operator of the PCS within the class of nonlinear operators is based on the concept of a penalty function for the error and is formulated as Bayes' approach to solving identification problems. The use of the error penalty as a characteristic of the deviation of the estimate from the true value of the variable expectation value leads to two important types of estimates: the a posterior probability (APP) and the maximum likelihood (ML), the relationship between which is expressed by Bayes' formula.

Depending on the method of minimizing the APP or ML penalty functions, the computational methods of identification are divided into two groups: direct and indirect. The first group includes those methods involving direct minimization of the penalty function at each step of the observation interval, specifically: the gradient method and its many variations, the method of stochastic approximation, etc. The second approach to solving the identification problem consists of using the principles of control theory at each iteraction step. In particular, Pontryagin's maximum principle, the method of Langrangian multipliers, etc., are used to minimize penalty functions. Here, the corresponding system of canonical equations with the necessary boundary conditions constitutes a typical nonlinear two-point (beginning or end of observation interval) boundary problem (TPBP), the solution of which is the value sought for the assigned observation interval. The computational methods used to solve the above TPBP constitute the group of so-called indirect computational methods of solving identification problems. This group includes the method of quasilinearization, the method of invariant immersion, the trial run method, etc.

The above scheme for solving the identification problem is by no means universal. It has serious limitations having to do with those assumptions set forth in the original formulation of the problem. Among typical situations to which the above scheme is inapplicable are: where the unknown parameters are not constant, but "drift" over time; where a priori information is lacking on the dispersion of the measurement errors; where object noises and measurement interferences are random processes different from white noise; where object noises represent the realization of nonsteady random processes; where object noises and measurement interferences correlate, etc. The above situations are especially characteristic of processes in the chemicals industry. Practically each of the above instances of a complication of the identification problem requires the use of special methods and procedures, the choice of which depends to a large degree on the specific conditions of the problem.

One way of overcoming the difficulties arising in problems of evaluating state parameters and identifying mass exchange processes is the use of statistical dynamics, operating with integral operators and weight functions for the systems being studied. The integral form of relationship between the input and output signals, in terms of the weight function of the system, is advantageous both from the viewpoint of resistance to interferences and with regard to the efficiency of the computational procedures. It is a virtue of this approach to solving identification problems that it opens up the possibility of making broad use of the exceptional properties of analytic processes in synthesizing optimum operators of objects with a finite "memory." It should be noted that the requirement of linearity of the system in order to realize the method only slightly diminishes its generality. The method is applicable to a broad class of nonlinear objects in chemicals technology if the techniques of nonlinear transformations of random functions are used.

In conclusion, it should be noted that objects in the chemicals industry involving heat and mass transfer processes are characterized by a high degree of nonlinearity, a substantial degree of distribution of parameters in space and time, transience and mutual correlation of input noises and measurement interference, continuous drift of process indices, deformation of the physicochemical structure of the processes occurring in the objects, etc. The above factors are the source of serious problems that arise in solving problems of estimating state parameters and identifying the object on the basis of the standard methods recommended by the modern theory of dynamic systems and examined above.

For example, experience in the practical realization of problems of estimating state parameters and identifying chemical processes using Kahlman filters [10, 11] has made it possible to discover several important limitations of the above approach with regard to solving these problems in the area of chemicals technology. Such limitations may be traced in part to the use of differential operators to describe the system mathematically and the finite-difference approximations of these operators in numerical operations. The realization of mathematical models such as these on a computer using the methods of formal algebra under conditions of high noise levels and rough initial estimates of state parameters is often associated with poor matrix conditionality and, thus, with instability and poor convergence in the computing procedures.

The questions involved in the study of the stability and convergence of computations in problems of identification and estimates of state parameters are so extensive and difficult that they now constitute an independent problem in and of themselves and entail the development of special methods and techniques for overcoming the aforementioned difficulties. Such methods and techniques include quasilinearization, stochastic approximation, invariant immersion, the gradient method and its many variants, etc. However, the use of these formal mathematical procedures by no means mitigates the very stringent requirements with respect accuracy in assigning the initial conditions on the state parameters and the initial estimates of the sought constants of the models, as well as with regard to the level of object noise and measurement interference. Additional complications arise in the case of transience and correlation and non-Gaussian nature of the noises, as is characteristic of objects in the chemicals industry. Thus, in solving problems of identification and estimating stateparameters for chemical industry processes, it would be expedient to make broader use of the possibilities offered by the formal apparatus of statistical dynamics and the theory of random functions on the basis of the use of integral operators and weight functions of the systems being investigated. It is important to emphasize that, in many cases, the weight function of an object in chemical technology is a function of the distribution of the time of residence of the particles of the substance in the production unit and is therefore a natural characteristic of the object [12, 13].

NOTATION

In Eqs. (3) and (4): ρ_{1k}^{o}, ρ_{2k}^{o}, true density of the k-th component in phases 1 and 2; $\rho_1^{o} = \sum_{k=1}^{n} \rho_{1k}^{o}$; ρ_2^{o}, true density of phases 1 and 2; $\rho_{1k} = \alpha_1 \rho_{1k}^{o}$; $\rho_{2k} = \alpha_2 \rho_{2k}^{o}$; $\rho_1 = \alpha_1 \rho_1^{o}$; $\rho_2 = \alpha_2 \rho_2^{o}$, mean density of the k-th component in phases 1 and 2 and the mean density of phases 1 and 2; α_1 and α_2, volume contents of phases 1 and 2; $\mathbf{v}_1 = \frac{1}{\rho_1} \sum_{k=1}^{n} \mathbf{v}_{1k}\rho_{1k}$; $\mathbf{v}_2 = \frac{1}{\rho_2} \sum_{k=1}^{n} \mathbf{v}_{2k}\rho_{2k}$, mean mass rates of phases 1 and 2; $\mathbf{v}_{ik}$, velocity of the k-th component in the i-th phase; $J_{k(12)}$, $J_{k(21)}$, "observed" macroscopic rates of interphase transfer of the k-th component in the directions 1 → 2 and 2 → 1; $J_{(21)} = \sum_{k=1}^{n} J_{k(21)}$; $J_{(12)} = \sum_{k=1}^{n} J_{k(12)}$; $J_{(1r)}$, $J_{(2r)}$, rates of the r-th reaction in the volume of phases 1 and 2 ($r = 1, 2, \ldots, N$); $\nu_{k(1r)} = \beta_{k(1r)} M_k$; $\nu_{k(2r)} = \beta_{k(2r)} M_k$; $\beta_{k(1r)}$; $\beta_{k(2r)}$, stoichiometric coefficients for the k-th component participating in the r-th reaction in phases 1 and 2; M_k, molecular weight of the k-th component; a is the number of particles; P, pressure; τ_1^{ql}, e_1^{ql}, components of the stress and strain tensors ($q, l = 1, 2, 3$); $\mathbf{f}_{(1r)}$ mass force due to the interaction between phases and including three effects (Stokes friction force, effect of virtual mass, Zhukovskii force); $\mathbf{v}_{(21)}$, $\mathbf{v}_{(12)}$, mean mass rates of the masses crossing the phase boundary in the directions 2 → 1 and 1 → 2; $\mathbf{F}_{1k}$, $\mathbf{F}_{2k}$, external mass forces acting on the particles of the k-th component in phases 1 and 2; $\mathbf{F}_1 = \sum_{k=1}^{n} \mathbf{F}_{1k}$; $\mathbf{F}_2 = \sum_{k=1}^{n} \mathbf{F}_{2k}$; u_1 and u_2, specific energy of phases 1 and 2; $\varkappa_1$ and $\varkappa_2$, fraction of kinetic energy of the mixture dissipated by the forceful interaction of the phases into the form of internal energy of phases 1 and 2 ($\varkappa_1 + \varkappa_2 = 1$); i_1 and i_2, specific enthalpy of phases 1 and 2; $i_{1k,s}$, $i_{2k,s}$, enthalpy of the k-th component in phases 1 and 2 at equilibrium; $q_{(21)}$, heat flux in contact heat exchange between the phases; $\mathbf{q}_1$ and $\mathbf{q}_2$, heat flux in phases 1 and 2; Q_1 and Q_2, power of the external heat sources; c_f, form factor of the particles; η, observed rate of change in the volume r of the particles ($0 < r \leq R$); c, mass concentration of the dissolved substance, calculated from the anhydrous product; m, ratio of the molecular weights of the anhydrous salt to the crystalline hydrate; f, particle size (volume) density function relative to a unit volume of the mixture; q_{tru}, density (power) of the source (sink) of particles of volume r; u_σ^1, surface energy associated with one inclusion; $q_{1\sigma}$, $q_{2\sigma}$, heat fluxes, relative to a unit volume of the mixture, from the carrier and r-th phases to the phase boundary; Q_1^* and Q_2^*, external flow of heat to the carrier and r-th phases; i_1 and i_2, specific enthalpies of the carrier and r-th phases; λ, thermal conductivity; β_i, coefficient of heat transfer from the i-th phase to the phase boundary; T_1, T_2, T_σ, temperature of the carrier phase, dispersed phase, and phase boundary (at the surface of the crystal).

LITERATURE CITED

1. V. V. Kafarov and I. N. Dorokhov, Systems Analysis of Chemical Industry Processes. Principles of Strategy [in Russian], Nauka, Moscow (1976).
2. V. V. Kafarov and I. N. Dorokhov, Systems Analysis of Chemical Industry Processes. Topological Principle of Formalization [in Russian], Nauka, Moscow (1979).

3. V. V. Kafarov, I. N. Dorokhov, and E. P. Markov, "Principle of describing chemical engineering processes by means of imperfect sets," Dokl. Akad. Nauk SSSR, 243, No. 1, 159-162 (1978); 246, No. 4, 931-934 (1979).
4. V. V. Kafarov, I. N. Dorokhov, and A. A. Dudorov, "Modeling physicochemical processes in polydispersed media on the basis of methods of statistical mechanics," Dokl. Akad. Nauk SSSR, 218, No. 4, 900-903 (1974).
5. I. N. Dorokhov, V. V. Kafarov, and R. I. Nigmatulin, "Methods of continuum mechanics for describing multiphase multicomponent mixtures with chemical reactions and heat and mass transfer processes," Prikl. Mat. Mekh., 39, No. 3, 485-497.
6. I. N. Dorokhov, V. V. Kafarov, and É. M. Kol'tsova, "Equations of the thermohydrodynamics of a two-phase polydispersed medium with phase changes with a continuous particle-size distribution," Prikl. Mekh. Tekh. Fiz., No. 1, 103-110 (1978).
7. V. V. Kafarov, Methods of Cybernetics in Chemistry and Chemical Engineering [in Russian], Khimiya, Moscow (1976).
8. V. V. Kafarov, Principles of Mass Transfer [in Russian], Vysshaya Shkola, Moscow (1979).
9. V. V. Kafarov, V. A. Klipinitser, N. G. Belyakov, and S. I. Smurov, "On the effect of the coefficient of molecular diffusion on mass transfer to the liquid phase in gas-liquid systems," Dokl. Akad. Nauk SSSR, 238, No. 1, 170-174 (1978).
10. V. V. Kafarov, I. N. Dorokhov, and A. N. Spiridonov, "New method of identifying mathematical models of chemical industry processes," Dokl. Akad. Nauk SSSR, 211, No. 4, 912-915 (1973).
11. V. V. Kafarov, I. N. Dorokhov, and A. N. Spiridonov, "New method of estimating state parameters of chemical industry processes," Dokl. Akad. Nauk SSSR, 211, No. 2, 400-404 (1973).
12. V. V. Kafarov, I. N. Dorokhov, and L. N. Lipatov, "Statistical method of checking hypotheses on the hydrodynamic structure of flows in production units," Dokl. Akad. Nauk. SSSR, 220, No. 5, 1145-1148 (1975).
13. V. V. Kafarov, I. N. Dorokhov, and L. N. Lipatov, "Method of estimating state parameters of chemical industry processes on the basis of object weight functions," Dokl. Akad. Nauk SSSR, 228, No. 5, 1151-1154 (1976).