A new Approach to Modeling and Simulation of Industrial Processes

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Abstract. *In the paper are presented theoretical analysis of the methods for industrial processes modeling and a new approach to modeling and simulation of industrial processes in cases of lack of information on the mechanism of the process.*
KEYWORDS: *MODELING, SIMULATION, CHEMICAL ENGINEERING, INDUSTRIAL PROCESSES*

Prelude

The main problems in the industry are the optimal design of new devices and the optimal control of active processes, i.e., minimization of the investment and operating costs. These problems are solved by modeling methods [1].

The creation of the mathematical model begins with the formulation of the physical model of the complex process, i.e., the definition of the simple (elementary) processes that make it up and the interactions between them. The second step is to define simple processes that have mathematical descriptions (equivalent mathematical operators). The other simple processes are introduced into the mathematical model through quantitative information obtained from experimental data, which brings the mathematical model as close as possible to the real process. The experiment brings mathematics closer to physics (reality).

The optimal design and control in the chemical industry is uniquely related to processes rates, so all mathematical descriptions of processes are linked to algorithms to determine these rates, i.e., processes kinetics.

Industrial Processes Kinetics

The industrial systems consist of separate phases (gas, liquid, solid) in the industrial apparatuses volumes. They are in thermodynamic equilibrium when the temperatures and concentrations of substances in the individual parts or points of the phases are equal and the velocities are equal to zero.

The processes in the industry are a result of the deviation of the systems from their thermodynamic equilibrium [2]. One system is not in a thermodynamic equilibrium when the velocities, concentrations of the components (substances) and the temperatures at the individual points in the phase volumes are different. These differences are the result of reactions, i.e., of processes that create or consume substance and (or) heat. As a result, the industrial processes kinetics is equivalent to the reactions kinetics [3].

The presented analysis shows that processes in the industry are result of reactions that occur in the phase volume (homogeneous) or on the boundary between two phases (heterogeneous). Homogeneous reactions are generally chemical, while heterogeneous reactions are chemical, catalytic, physical and chemical adsorption, interphase mass transfer in gas-liquid and liquid-liquid systems (on the interphase surface the substance disappears from one phase and occurs in the other phase). The rates of these processes are determined by the reaction kinetics [3], which lies at the basis of modeling and simulation of the industrial processes.

Modeling

The basics of modeling in chemical engineering, as part of human knowledge and science, are related to the combination of intuition and logic that has different forms in individual sciences [4]. In the mathematics the intuition is the axiom (unconditional statements, that cannot be proven), while the logic is the theorem (the logical consequences of the axiom), but logic prevails over intuition. In the natural sciences (physics, chemistry, biology), the "axioms" (principles, postulates, laws) are not always unconditional, but logic prevails over intuition too.

The processes in the industry take place in the industrial apparatuses, where gas, liquid and solid phases move together or alone. They are described by variables, which are extensive or intensive. In the case of merging of two identical systems, the extensive variables are doubled, but the intensive variables are retained.

In the industry, processes take place in moving phases (gas, liquid, solid). Reactions (reaction processes) lead to different concentrations (and temperatures) in the phase volumes and the phase boundaries. As a result, hydrodynamic processes, diffusion mass transfer and heat conduction are joined to the reaction processes. Under these conditions there are various forms of mass transfer (heat transfer) that are convective (as a result of phase movements) and diffusion (as a result of concentration (temperature) gradients in the phases).

Convective mass transfer (heat transfer) can be laminar or turbulent (as a result of large-scale turbulent pulsations). Diffusion mass transfer (heat transfer) can be molecular or turbulent (as a result of small-scale turbulent pulsations).

Mathematical models of industrial apparatuses aim at determining the concentration of substances (flow temperatures) in the phases. They have different degrees of approximation – thermodynamic, hydrodynamic and Boltzmann's approximations.

Thermodynamic Approximation

The processes in chemical engineering are result of a deviation from the thermodynamic equilibrium between two-phase volumes or the volume and phase boundaries of one phase and represent the pursuit of systems to achieve thermodynamic equilibrium [2]. They are irreversible processes and their kinetics use mathematical structures derived from Onsager's principle of linearity (axiom). According to him, the average values of the derivatives at the time of the extensive variables depend linearly on the mean deviations of the conjugated intensive variables from their equilibrium states. The principle is valid close to equilibrium, and the Onsager's linearity coefficients are kinetic constants. When the process is done away from equilibrium (high intensity processes) kinetic constants become kinetic complexes, depending on the corresponding intensive variables. The thermodynamic approximation models cover the entire volume of the phase or part of it.

Hydrodynamic Approximations

The hydrodynamic level uses the approximations of the mechanics of continua, where the mathematical point is equivalent to an elementary physical volume, which is sufficiently small with respect to the apparatus volume, but at the same time sufficiently large with respect to the intermolecular volumes in the medium. In this level the molecules are not visible, as is done in the next level of detail of Boltzmann.

The models of the hydrodynamic approximations are possible to be created on the basis of the mass (heat) transfer theory, whose models are created by the models of the hydrodynamics, diffusion, thermal conductivity and reaction kinetics, using the logical structures of three main “axioms”, related with the impulse, mass and heat transfer:

1. The postulate of Stokes for the linear relationship between the stress and deformation rate, which is the basis of the Newtonian fluid dynamics models;
2. The first law of Fick for the linear relationship between the mass flow and the concentration gradient, which is the basis of the linear theory of the mass transfer;

3. The first law of Fourier for the linear relationship between the heat flux and the temperature gradient, which is the basis of the linear theories of the heat transfer.

These are the laws of the impulse, mass and energy transfer.

To the above axioms must be added the law of chemical kinetics - the rate of two-molecular reactions depends linearly on the product of the concentrations of the reagents. This law is not an axiom because it follows from the rule of probabilities. The reaction between two molecules takes place when they are at one point. The probability that a molecule of a reagent is at a given point is equal to the ratio of the number of its molecules and the total number of molecules, i.e, it is proportional to its concentration. The same is true for the second reagent. The simultaneous realization of both probabilities is the complex probability, which is equal to the product of the simple probabilities.

Boltzmann's Approximation

In Boltzmann's kinetic theory of the ideal gas, the hydrodynamic "axioms" are three "theorems" that derive from the axiom of the "elastic shock" (in a shock between two molecules the direction and the velocity of the movement change, but the sum of their kinetic energies is retained, i.e., there is no loss of kinetic energy) and the rate coefficients are theoretically determined by the average velocity and the average free run of the molecules.

Mechanism of Influence of Reaction Kinetics

The mathematical model of an engineering process is a mass (heat) balance in the phases volumes, where the mathematical operators are mathematical descriptions of the composite (elementary) processes, and the relationship between them (differential equations) corresponds to the mechanism of the complex process. The boundary conditions of the differential equations are formulated at the interphase boundaries.

Industrial processes are a set of physical and chemical reactions, hydrodynamic, diffusion and thermal processes that take place in the industrial apparatus volume. The problems in the modeling of the kinetics of industrial processes arise from the need for information about the interaction between the simple (elementary) processes in the complex process, i.e., information about the process mechanism.

Modeling of Processes with Unknown Mechanism

There are complex processes whose mechanism is unknown. A typical example of this are the complex chemical reactions, where the rate of which depends on the concentrations of several substances, but the simple chemical reactions between these substances and the relationships between them are unknown.

The kinetics of processes with an unknown mechanism can be modeled on the basis of an axiom, which can be formulated as it - "The mathematical structure of the quantitative description of real (industrial) processes does not depend on the measuring system of the quantities involved in them".

A. A. Gukhman formulates [8] the condition for homogeneity of a function – „The function in the equation $F\left(x_1,...,x_n\right)=0$ is homogeneous, if is invariant $F\left(k_1x_1,...,k_nx_n\right)=0$ with respect to similar transformations $x_i=k_ix_i, i=1,...,n$ ($k_i, i=1,...,n$ - positive constants)", i.e.,

$$F\left(k_1x_1,...,k_nx_n\right)=\varphi\left(k_1,...,k_n\right)F\left(x_1,...,x_n\right). \quad (1)$$

The homogeneous functions satisfy the equation (1) in the cases $F\left(x_1,...,x_n\right)\neq 0$, too.

Using the equation (1), Gukhman formulates and proves the theorem [5] – "If mathematical structure is invariant with respect to similar transformations, it is possible to be presented as power functions complex". This Gukhman's theorem can be considered as a consequence of the axiom „Mathematical structure of real process does not depend on the measuring system", because the mathematical structure, which is invariant with respect to similar transformations is mathematical structure of real processes, which does not depend on the measuring system. As a result is possible to be formulate the theorem „Mathematical structure of the quantitative description of real systems is possible to be presented as power functions complex". This theorem will be proved for cases of complex chemical reactions.

The kinetics of the complex chemical reactions depends on a set of variables. If the velocity of these processes is denoted by y and the values of these variables are $x_1,...,x_n$, the equation of the kinetic model will have the form:

$$y=f\left(x_1,...,x_n\right). \quad (2)$$

This function is a mathematical structure that is retained when changed the measurement system of the variable, i.e., this mathematical structure is invariant with respect to similar transformations [5]:

$$\overline{x}_i=k_ix_i, \quad i=1,...,n, \quad (3)$$

i.e., f is a homogeneous function:

$$ky=f\left(k_1x_1,...,k_nx_n\right)=\phi\left(k_1,...,k_n\right).f\left(x_1,...,x_n\right), \quad k=\phi\left(k_1,...,k_n\right). \quad (4)$$

A short recording of (4) is:

$$f\left[\overline{x}_i\right]=\phi\left[k_i\right]f\left[x_i\right]. \quad (5)$$

The problem consists in finding a function *f* that satisfies equation (5). A differentiation of equation (5) concerning k_1 leads to:

$$\frac{\partial f\left[\overline{x}_i\right]}{\partial k_1}=\frac{\partial \phi}{\partial k_1}f\left(x_i\right). \quad (6)$$

On the other hand

$$\frac{\partial f\left[\overline{x}_i\right]}{\partial k_1}=\frac{\partial f\left[\overline{x}_i\right]}{\partial \overline{x}_1}\frac{\partial \overline{x}_1}{\partial k_1}=\frac{\partial f\left[\overline{x}_i\right]}{\partial \overline{x}_1}x_1. \quad (7)$$

From (6, 7) follows

$$\frac{\partial f\left[\overline{x}_i\right]}{\partial \overline{x}_1}x_1=\alpha_1 f\left[x_i\right], \quad (8)$$

where

$$\alpha_1=\left(\frac{\partial \phi}{\partial k_1}\right)_{k_i=1}. \quad (9)$$

The equation (8) is valid for different values of k_i including $k_i=1 \ \left(i=1,...,n\right)$. As a result $\overline{x}_i=x_i, i=1,...,n$ and from (8) follows

$$\frac{1}{f}\frac{\partial f}{\partial x_1}=\frac{\alpha_1}{x_1}, \quad (10)$$

i.e.

$$f = c_1 x_1^{\alpha_1}. \quad (11)$$

When the above operations are repeated for $x_2,...,x_n$, the homogenous function *f* assumes the form:

$$f = k x_1^{\alpha_1},...,x_n^{\alpha_n}, \quad (12)$$

i.e. the function *f* is homogenous if it represents a power functions complex and as a result is invariant with respect to similarity (metric) transformations. The parameters $k,\alpha_1,...,\alpha_n$ are determined by experimental data of the industrial process velocity.

Parameters Identification

The parameters $k,\alpha_1,...,\alpha_n$ identification in (12) uses experimental data of the industrial process velocity $f_j^{\exp}$, $j=1,...,N$ for different values of the variables are $x_{1j},...,x_{nj}$, $j=1,...,N$, where the calculated values of the industrial process velocity are

$$f_j = k x_{1j}^{\alpha_1},...,x_{nj}^{\alpha_n}, \quad j=1,...,N. \quad (13)$$

The parameters identification of the model requires its preliminary logarithmization

$$F_j = \alpha_0 + \alpha_1 X_{1j},...,\alpha_n X_{nj}, \quad j=1,...,N, \quad F=\log f, \quad \alpha_0 = \log k, \quad X = \log x \quad (14)$$

The differences between the calculated and experimental values of the industrial process velocity will be presented as

$$\alpha_0 + \alpha_1 X_{1j},...,\alpha_n X_{nj} - F_j^{\exp} = \varepsilon_j, \quad j=1,...,N, \quad F_j^{\exp} = \log f_j^{\exp} \quad (15)$$

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The solution of the parameters identification problem can be obtained as a minimization of the least-squares function:

$$Q(\alpha_0,\alpha_1,...,\alpha_n) = \sum_{j=1}^{N}\left(\alpha_0 + \alpha_1 X_{1j},...,\alpha_n X_{nj} - F_j^{\exp}\right)^2, \quad (16)$$

using the condition

$$\frac{\partial Q}{\partial a_i} = 0, \quad i = 0,1,...,n \quad , (17)$$

i.e.

$$\sum_{j=1}^{N} 2\left(\alpha_0 + \alpha_1 X_{1j},...,\alpha_n X_{nj} - F_j^{\exp}\right) = 0,$$

$$\sum_{j=1}^{N} 2\left(\alpha_0 + \alpha_1 X_{1j},...,\alpha_n X_{nj} - F_j^{\exp}\right) X_{1j} = 0,$$

$$\sum_{j=1}^{N} 2\left(\alpha_0 + \alpha_1 X_{1j},...,\alpha_n X_{nj} - F_j^{\exp}\right) X_{2j} = 0, , \quad (18)$$

...

$$\sum_{j=1}^{N} 2\left(\alpha_0 + \alpha_1 X_{1j},...,\alpha_n X_{nj} - F_j^{\exp}\right) X_{nj} = 0.$$

The solution of the equation set (18) permits to be obtained the parameters values in the model (12). Determining parameter $\kappa = 10^{\alpha_0}$ by antilogarithmization of parameter α_0 is not recommended due to increasing computational error of α_0. The equation (13) can be used for this purpose:

$$k = \frac{1}{N}\sum_{j=1}^{N} \frac{f_j}{x_{1j}^{\alpha_1},...,x_{nj}^{\alpha_n}}. \quad (19)$$

Presented algorithm (13-19) permits to use power functions complex (12) as an universal model of the real (industrial) processes.

Conclusions

In the paper is presented a theoretical analysis of the methods for industrial processes modeling.

The role of the kinetics of industrial processes for solving the problems of optimal design and control is analyzed. The thermodynamic, hydrodynamic and Boltzmann approximations for the mathematical description of the kinetics of industrial processes are described.

A new approach to modeling of industrial processes with unknown mechanism is presented on the base of formulated axiom and theorem. The axiom „Mathematical structure of real process does not depend on the measuring system“ is used for the formulation of the theorem “Mathematical structure of the quantitative description of real systems is possible to be presented as power functions complex”.

An algorithm, for the parameters identification in the power functions complex model, permits to modeling and simulation of industrial processes.

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