Introduction in the Chemical Engineering Processes Modeling

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In the paper is presented a theoretical analysis of the methods for chemical engineering processes modeling. The methods for modeling specific processes may be different, but in all cases they must bring the mathematical description closer to the real process by using appropriate experimental data. These methods are presented in the cases of co-current absorption column without packings, counter-current absorption column with random packings and modeling of processes with unknown mechanism.

The main problems in the chemical industry (biotechnology, heat energy) 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 chemical engineering with modeling methods.

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 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.

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

The processes in the chemical industry (biotechnology, heat energy) are a result of the deviation of the systems from their thermodynamic equilibrium. 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.

The presented analysis shows that processes in the chemical 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, which lies at the basis of modeling in chemical engineering, and solving the basic problems in the chemical industry (biotechnology, heat energy).

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. 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 chemical engineering 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 chemical industry (biotechnology, heat energy), 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.

The processes in chemical engineering are the 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. They are irreversible processes and their kinetics use mathematical structures derived from Onsager's principle of linearity. 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.

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 diffusion 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.

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.

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