Journal of Clinical Chemistry and Laboratory Medicine

OPEN ACCESS Freely available online

Research Article

Introduction in the Chemical Engineering Processes Modeling

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ABSTRACT

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.

Keywords: Chemical engineering; Physics; Algorithms

INTRODUCTION

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 [1]. The processes in the chemical industry (biotechnology, heat energy) 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 heat. As a result the industrial processes kinetics is equivalent to the reactions kinetics [3]. 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 [3], 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 [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 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

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Received: February 10, 2021; **Accepted**: February 24, 2021; **Published**: March 1, 2021

Citation: Boyadjiev C (2021) Introduction in the Chemical Engineering Processes Modeling. J Clin Chem Lab Med. 5: 160.

approximation – thermodynamic, hydrodynamic and Boltzmann's approximations.

The prevalence of diseases in society can serve as an indicator. How well society will do appears to depend on it. By all indications, the US has failed to contain a deadly virus such as Covid-19. As of December 21 according to the John Hopkins University and Medicine, Coronavirus Resource Center reports that the US has over 17 million infection cases and over 318,000 deaths due to Covid-19. It ranks 13th among nations with the highest, with 97 per 100,000 [5]. Except for Peru, all other nations listed with higher rates are either Western or Eastern European (e.g., San Mario, Belgium, Peru, Slovenia, Italy, N. Macedonia, Bosnia, Spain, Andorra, the UK, Montenegro, and Czech Rep). The one similarity with all of these nations is that they are all fully integrated into the world capitalist system.

THERMODYNAMIC APPROXIMATION

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 [2]. 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 [6].

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 [7].

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: The postulate of Stokes for the linear relationship between the stress and deformation rate, which is the basis of the Newtonian fluid dynamics models; 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; 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 [8].

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 [9].

The mathematical model of an engineering chemical process is a mass (heat) balance in the phases volumes, where the mathematical operators are mathematical descriptions of the composite 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. For this purpose, the knowledge of the mathematical descriptions of the velocity distribution in the phases and the interphase boundaries is necessary. 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 compiling the models of the kinetics of industrial apparatuses arise from the need for information about the interaction between the individual processes in the complex process (its mechanism) and a mathematical description of the geometry of the industrial apparatus volume. For the most part, industrial cases do not have the above information, which requires simplification of the models and introduction of some effects through experimentally determined parameters. As example will consider a co-current absorption column without packings and a counter current absorption column with random packings [10].

CO-CURRENT ABSORPTION COLUMN WITHOUT PACKINGS

In the absorption columns without packings, the velocity distributions in the gas and liquid phases and the interfacial limits are unknown, i.e. the differential equations (mass balances in the phases) and their boundary conditions at the interphase boundaries (velocity of the interphase mass transfer) cannot be formulated. These problems are overcome by creating of convection-diffusion and average-concentration models [5,6]. In the convection-diffusion model the velocity of the interphase mass transfer is replaced by volume physical reaction and experimentally determinable parameter. In this model, the velocities are unknown, so it can only be used for qualitative analysis. From it the average-concentration models are obtained, by model averaging along the cross section of the column. The obtained average-concentration model involves average velocities and concentrations, and the velocity distributions in the phase volumes are introduced with experimentally determined parameters.

FLUID FLOW ALONG THE COLUMN WALL

The liquid flow on the surface of the random packings and when it reaches the column wall most of it flows on this surface and cannot return to the column volume due to the small contact surface between the wall surface and the random packings. The thickness of the flowing layer of liquid increases and conditions are created for the return of liquid from the layer to the packings and further the two effects are equalized. In this way, the layer of liquid reaches a constant maximum thickness, with which it moves to the end of the column. The amount of liquid entering the flowing layer leads to a reduction in the amount of liquid in the volume of the column, i.e. to the radial non-uniformity of the axial component of the liquid velocity in the column and to the reduction of the mass transfer rate in the liquid phase. In addition, this layer is not involved in the absorption process.

The effect of liquid flowing on the column wall is the result only of the geometric shape of the random packings and thus determines the rate of absorption of slightly soluble gases, which reaches a maximum value at maximum packings surface per unit volume of the column and minimum thickness of the flowing layer of liquid.

CONCLUSION

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. The role of the kinetics of industrial apparatuses 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 apparatuses are described. They are presented the cases of co-current absorption column without packings, counter-current absorption column with random packings and modeling of processes with unknown mechanism.

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