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Biotechnology Reactions Kinetics

Abstract

In the paper is presented a theoretical analysis of the role of the reaction kinetics in biotechnology(chemical engineering, heat energy)for the solution of the main industrial problems, i.e. the optimal design of new devices and the optimal control of active processes. The thermodynamic and hydrodynamic approximations for the modeling of the industrial process rates are presented and analyzed.

Keywords

Reaction Kinetics; Optimal Design; Optimal Control; Thermodynamic Approximation; Hydrodynamic Approximation

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Christo Boyadjiev*

Institute of Chemical Engineering, Bulgarian Academy of Sciences

***Address for Correspondence**

Christo Boyadjiev, Institute of Chemical Engineering, Bulgarian Academy of Sciences, Bulgaria

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Introduction

The main problems in the biotechnology (chemical engineering, 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 modeling and simulation methods. Mathematical models of processes in the industry *[1]* contain equations, involving variables and parameters. Depending on the problem solved, variables can become parameters and vice versa. They are input mode variables (X), output mode variables (Y), and construction parameters (A):

$$F(X,Y,A)=0, \quad (1)$$

where F is a "vector", containing all the equations in the model, $X(Y)$ are the vectors of the input (output) variables, that contain the flow rates and temperatures of the input (output) phase flows and the concentrations of their components, A is the vector of the constructive parameters, which contains the constructive parameters of the apparatuses.

The solutions to the optimal design problems of new apparatuses use algorithms, where input mode variables (X) and output mode variables (Y) are set (as parameters) and optimal construction parameters must be obtained (as variables):

$$A=F_1(X,Y). \quad (2)$$

The problems of optimal control of current processes use algorithms, where the output mode variables (Y) and constructive parameters (A) are set (as parameters) and the optimal input mode variables (X) are searched:

$$X=F_2(Y,A). \quad (3)$$

In the case of renovation (optimal reconstruction), part of the input mode variables and construction parameters are set. Optimal design and control in the chemical industry is uniquely related to process rates, so all mathematical descriptions of processes are linked to algorithms to determine these rates.

The processes rates in the Industrial Processes

The processes in the biotechnology (chemical engineering, heat energy) are the result of the deviation of the systems from their thermodynamic equilibrium *[2]*. One system is not in a thermodynamic equilibrium when the concentrations of the components (substances) and the temperature 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. 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 biological and 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 and simulation in biotechnology.

Modeling and Simulation

The basics of modeling and simulation in biotechnology, as part of human knowledge and science, are related to the combination of intuition and logic that has different forms in

individual sciences [3]. 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 biotechnology 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. The processes in the 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 the systems to achieve the thermodynamic equilibrium. They are irreversible processes and their kinetics use mathematical structures derived from Onsager's principle of linearity *[2]*. 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 near equilibrium and the proportionality factors are the kinetic constants. When the process is done away from equilibrium (high intensity processes) kinetic constants become kinetic complexes, depending on the corresponding intensive variables.

Mechanism of Influence of Reaction Kinetics

In the biotechnology (chemical industry, 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 processes aim at determining the concentration of substances (flow temperatures) in the phases. Mathematical models represent a material (thermal) balance in an elementary (small) phase volume that is equivalent to a mathematical point. Components in this balance are convective mass transfer (heat transfer), diffusion mass transfer (heat transfer) and homogeneous reactions (heat effect of reactions). Heterogeneous reactions take part in the boundary conditions of the equations in mass transfer (heat transfer) models. On this basis models of classical theory of mass transfer were created.

Theory of Mass Transfer

The modern theory of mass transfer is based on the theory of the diffusion boundary layer *[4,5]* (Landau, Levich). This approach replaces (physically justified) elliptic partial differential equations with parabolic partial differential equations, which facilitates their mathematical solution and offers a mathematical description of physical processes with free (not predetermined) ends. The theory of the diffusion boundary layer develops in the case of drops and bubbles *[5]* (Levich, Krylov), liquid film flows *[6]* (Levich, Krylov, Boyadjiev, Beschkov), non-linear mass transfer and hydrodynamic stability *[7,8]* (Krylov, Boyadjiev, Babak). The modeling of chemical engineering processes has two levels of detail - thermodynamic and hydrodynamic approximation.

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. 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.

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 diffusion and reaction kinetics, using the logical structures of three main "axioms", related with the impulse, mass and heat transfer:

a) The postulate of Stokes for the linear relationship between the stress and deformation rate, which is the basis of the Newtonian fluid dynamics models;

b) 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;

c) 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, these 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.

Conclusion

The main problems in the biotechnology (chemical industry, heat energy) are the optimal design and optimal control of the industrial processes, using the laws of the reaction kinetics. Industrial processes are the result of reactions, i.e. creation or disappearance of a substance and (or) heat as a result of biological, chemical and (or) physical processes and their rate is determined by the reaction kinetics. The reactions deviate the systems from the thermodynamic equilibrium and as a result processes arise, who are trying to restore that equilibrium. The rate of these processes can be determined by Onsager's "linearity principle", where the rate of the process depends linearly on the deviation from the thermodynamic equilibrium.

References

1. Chr Boyadjiev (2010) Theoretical Chemical Engineering. Modeling and simulation, Springer-Verlag, Berlin Heidelberg.
2. J Keizer (1987) Statistical Thermodynamics of Nonequilibrium Processes, Springer-Verlag, New York, USA.
3. Chr Boyadjiev (2014) Open Access Library Journal 6(1).
4. LD Landau (1989) EM Lifshitz, Fluid Mechanics, Pergamon, Oxford, USA.
5. VG Levich (1962) Physicochemical Hydrodynamics, Prentice Hall, New York, USA.
6. Chr Boyadjiev, V Beschkov (1984) Mass Transfer in Liquid Film Flows, Publ House Bulg Acad Sci Sofia.
7. ВС Крылов,Хр.Бояджиев,НелинейныйМассоперенос, Изд. Институт теплофизики СОРАН, Новосибирск,1996.
8. Chr B Boyadjiev, VN Babak (2000) Non-Linear Mass Transfer and Hydrodynamic Stability, Elsevier, New York, USA.