

MODELING AND SIMULATION OF INDUSTRIAL PROCESSES

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Abstract: In the paper are presented the main theoretical techniques used for the modeling and simulation of industrial processes. The main focus is on the physical side of the theoretical techniques and their mathematical side is reduced to a reasonable minimum. Different theoretical approximations as thermodynamic and hydrodynamic levels are used.

KEYWORDS: MODELING, SIMULATION, THEORETICAL APPROXIMATION, THERMODYNAMIC LEVEL, HYDRODYNAMIC LEVEL, MECHANISM IDENTIFICATION, PARAMETERS IDENTIFICATION, STATISTICAL ANALYSIS.

1. Introduction

The modeling and simulation are a basic approach to quantifying processes and phenomena [1-3]. They have become realistic as a result of the development of computing and applied mathematics. In the industry, the modeling and simulation offer a quantitative description of the kinetics of processes and systems for the purposes of their optimal design or control. In the industrial systems, the process models of the individual devices are known in advance, and system models offer quantitative descriptions of the systems (process systems engineering).

In the industry, quantification of systems can also be used for various other tasks. For example, in periodically operating systems, the optimal schedules of the apparatuses (machines) for conducting different processes (operations) of different duration and different sequence to obtain different substances (machined details) can be determined. In these cases, the mass service theory offers models that allow for optimal solutions.

The fundamentals of the modeling and simulation, as a part of human knowledge and science, are related to the combination of intuition and logic. They are in different scales in the individual sciences [4, 5]. In the mathematics, logic dominates intuition, where intuition is the axiom (unconditional truth that is not proof able), and logic is the theorem (the logical consequences of the axiom). In the natural sciences (physics, chemistry, biology), the logic/intuition ratio is maintained, but axioms are usually conditional (principles, postulates, laws). This ratio goes back to the humanities and reaches the extreme in religion.

The modeling and simulation offer quantitative (mathematical) descriptions that have different degrees of detail. The lowest level is the thermodynamic (non-equilibrium thermodynamics) that examines the volume of the phase (gas, liquid, solid). The next level is the hydrodynamic, which examines the elementary phase volumes (mechanics of continua), which are much smaller than the phase volumes, but much larger than the intermolecular volumes, i.e. the molecules are indistinguishable. The highest level is the molecular (the kinetic theory of the ideal gas).

The modeling and simulation of industrial processes has a wide application, so the processes in the chemical industry and related biotechnologies and heating technologies, will be discussed. The major part of these processes is the transfer of mass and heat as a result of phase or phase boundary reactions. By reaction, will be understand the creation or disappearance of a particular substance (or amount of heat) as a result of a chemical reaction in the phase or on the phase boundary, interphase mass transfer, adsorption on the phase boundary or a liquid-vapor-liquid phase transition. These reactions result in varying concentrations and temperatures in the phases, i. e. to a deviation from the thermodynamic equilibrium and as a result of the mass transfer and heat transfer to restore the thermodynamic equilibrium. The models of the mass transfer and heat transfer are analogous and, therefore, the models of mass transfer in industrial processes will be presented.

2. Thermodynamic approximation

The reactions deviate the industrial systems from the thermodynamic equilibrium and the industrial processes for its recovery begin. The determining of the rate of these processes is a major problem in the industry, as it is the basis for their optimal design and control. This gives reason to use the thermodynamic laws of irreversible processes such as mathematical structures in the construction of the process models, described by extensive and

intense variables (in the case of merging of two identical systems, the extensive variables double their values, while the intensive variables retain their values).

The kinetics of the irreversible processes uses the mathematical structures, resulting from Onsanger's "linearity principle" [6]. According to him, the mean 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 (values). This principle is valid in the vicinity of the equilibrium, and proportionality coefficients are kinetic (rate) constants.

According to the principle of linearity, the mass derivative at time

$J_0 = \frac{dm}{dt}$ [kg-mol.s⁻¹] depends linearly on the deviation from the

thermodynamic equilibrium ΔC [kg-mol.m⁻³] of the concentration in two phase volumes or in one phase and the phase boundary, i.e.

$$J_0 = k_0 \Delta C, \quad (1)$$

where k_0 [m³.s⁻¹] is a proportionality coefficient.

Consider a system that contains two identical volumes in one phase $v_1 = v_2 = v$ [m³]. The system contains a substance whose masses

m_i [kg-mol] and concentrations $c_i = \frac{m_i}{v_i}$ [kg-mol.m⁻³] are

different in two volumes, $i = 1, 2, \dots$. The system is not in thermodynamic equilibrium. Let us assume for certainty

$c_1 - c_2 > 0$, $i = 1, 2$. As a result, the mass of the substance

starts to be transferred from volume v_1 to volume v_2 for to achieve the equilibrium. According to the principle of linearity, the mass transfer rate between the two volumes J_0 [kg-mol.s⁻¹] can be represented as:

$$J_0 = \frac{dm_1}{dt} = -\frac{dm_2}{dt} = k_0 (c_1 - c_2), \quad (2)$$

where k_0 [kg-mol⁻¹.m³.s⁻¹] is a proportionality coefficient. If we replace masses with concentrations $m_i = v_i c_i$, $i = 1, 2$, the mass

transfer rate in one phase J [kg-mol.m⁻³.s⁻¹] between two points with different concentrations is:

$$J = \frac{dc_1}{dt} = -\frac{dc_2}{dt} = k (c_1 - c_2), \quad (3)$$

where k [s⁻¹] is a rate coefficient. This equation is capable of presenting the rate of interphase mass transfer in the case of adsorption or catalytic process, where C_1 is the concentration of the substance in the gas phase, while C_2 is the concentration of the substance in the gaseous portion of the solid (capillaries of the adsorbent or catalyst) phase.

In the cases, where the volumes $v_1 = v_2 = v$ are in different phases (for example, 1 is a gas phase and 2 is a liquid phase), the

thermodynamic equilibrium law has the form $c_1 - \chi c_2 = 0$, i.e. this is the Henry's law and χ is the Henry's number. If $c_1 - \chi c_2 > 0$ the mass transfer is from phase 1 to phase 2 and the mass transfer rate between phases is:

$$J = k(c_1 - \chi c_2), \quad (4)$$

where k [s^{-1}] is the rate coefficient of the interphase mass transfer. On the surface between two phases, the thermodynamic equilibrium is immediately established, practically, i.e. $c_1^* - \chi c_2^* = 0$, where c_i^* , $i = 1, 2$, are the equilibrium concentrations on the phase boundary. Thus, the mass transfer rate can be expressed by mass transfer rate in two phases:

$$J = k_1(c_1 - c_1^*) = k_2(c_2^* - c_2), \quad (5)$$

where k_i , $i = 1, 2$ [s^{-1}] are mass transfer rate coefficients.

The Onsanger principle of linearity represents the thermodynamic approximation of the mathematical description of the kinetics of irreversible processes, but it does not show the way to reach equilibrium, i.e. the mechanism of the process and as a result the rate coefficient is not known. Obviously, this "thermodynamic level" does not allow a real quantitative description of the kinetics of irreversible processes in industry and the next level of detail of the description, the so-called "hydrodynamic level", should be used.

3. Hydrodynamic approximation

The processes in the chemical industry and related biotechnologies and heating technologies are realized in one-, two- and three-phase systems (gas-liquid-solid). They are a result from the reactions, i.e. processes of disappearance or creation of any substance. The reactions are associated with a particular phase and can be homogeneous (occurring in volume of the phase) or heterogeneous (occurring at the interface with another phase). Homogeneous reactions are usually chemical, while heterogeneous reactions may be chemical, catalytic and adsorption. Heterogeneous reaction is the interphase mass transfer too, where on the interphase boundary the substance disappears (created) in one phase and creates (disappears) in the other phase.

The volume reactions lead to different concentrations of the reagents in the phase volumes and as a result two mass transfer processes are realized – convective transfer (caused by the movement of the phases) and diffusion transfer (caused by the concentration gradients in the phases). The mass transfer models are a mass balance in the phases, where components are convective transfer, diffusion transfer and volume reactions (volume mass sources or sinks). The surface reactions participate as mass sources or sinks in the boundary conditions of the model equations. The models of this complex process are possible to be created on the basis of the mass transfer theory, whose models are created by the models of the hydrodynamics, diffusion and reaction kinetics. The mass transfer theory combines the chemistry, physics and mathematics and builds its logical structures on three main "axioms":

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, these axioms are replaced by the "elastic shock" axiom (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.

The contemporary mass transfer theory is based of diffusion boundary layer theory (Landau, Levich [7]). This approach substitutes (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 diffusion boundary layer theory is developed in the cases of drops and bubbles (Levich, Krylov [8]), film flows (Levich, Krylov, Boyadjiev, Beshkov[9, 10]), non-linear mass transfer and hydrodynamic stability (Krylov, Boyadjiev, Babak [11, 12]).

3.1. Mass transfer theory

The complex industrial processes are a collection of elementary physical and chemical processes. For example, the chemical absorption in a packed bed column represents a physical absorption of a gas phase component in the liquid phase and a subsequent chemical reaction with a component of the liquid phase. The gas moves in the column like jets and bubbles, while the liquid moves in the form of drops, jets, and flowing films on the surface of the packed bed. As a result, the chemical absorption in a packed bed column is a combination of many elementary physical and chemical processes, as absorption in the systems gas-liquid drops, liquid-gas bubbles, gas-liquid film flow, etc. As an example will be considered the gas absorption in liquid film with free interface.

Let us consider absorption of a slightly soluble gas in a laminar liquid film [9, 10] in a coordinate system (x, y) , flowing over a flat vertical interface $(y = 0)$. The hydrodynamic model has the form:

$$\nu \frac{\partial^2 u_x}{\partial y^2} + g = 0, \quad \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} = 0; \quad (6)$$

$$y = 0, \quad u_x = 0, \quad u_y = 0; \quad y = h_0, \quad \frac{\partial u_x}{\partial y} = 0$$

and the velocity distribution is:

$$u_x = \frac{g}{2\nu}(2h_0y - y^2), \quad u_y = 0. \quad (7)$$

If these conditions the convection-diffusion model has the form:

$$\frac{g}{2\nu}(2h_0y - y^2) \frac{\partial c}{\partial x} = D \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right),$$

$$x = 0, \quad c = c_0; \quad x \rightarrow \infty, \quad c = c^*; \quad (8)$$

$$y = 0, \quad \frac{\partial c}{\partial y} = 0; \quad y = h_0, \quad c = c^*,$$

where the thermodynamically equilibrium exists at the film interface $(y = h_0)$ and c^* denotes the equilibrium concentration.

The solid interface $(y = 0)$ is impenetrable for the diffusing substance with inlet concentration $c_0 < c^*$ (absorption). A film of length l will be considered.

The diffusion boundary layer thickness δ [2] is:

$$\delta = \sqrt{\frac{Dl}{u^*}} = \frac{l}{\sqrt{Pe}}, \quad Pe = \frac{u^*l}{D}, \quad \frac{\delta}{l} = \frac{1}{\sqrt{Pe}}, \quad u^* = \frac{gh_0^2}{2\nu}, \quad \frac{\delta^2}{h_0^2} = Fo = \frac{Dl}{u^*h_0^2}, \quad (9)$$

where u^* , Pe , Fo , are the film interface velocity, the Peclet and Fourier numbers.

The diffusion boundary layer thickness δ is less than liquid film thickness h_0 that permits the diffusion boundary layer

approximation to be applied. As a result, the next generalized variables can be introduced:

$$x = lX, \quad y = h_0 - \delta Y, \quad c = c_0 + (c^* - c_0)C, \quad (10)$$

where $0 = \frac{h_0}{l} \leq 10^{-2}$.

The introduction of (10) into (8) yields:

$$\begin{aligned} (1 + FoY^2) \frac{\partial C}{\partial X} &= \frac{Dl}{u^* \delta^2} \left(Pe^{-1} \frac{\partial^2 C}{\partial X^2} + \frac{\partial^2 C}{\partial Y^2} \right); \\ X = 0, \quad C = 0; \quad X \rightarrow \infty, \quad C = 1; \\ Y \rightarrow \infty, \quad C = 0; \quad Y = 0, \quad C = 1, \end{aligned} \quad (11)$$

where Fo is a small parameter:

$$\frac{\delta^2}{h_0^2} = Fo < 10^{-1}, \quad \frac{\delta^2}{l^2} = Pe^{-1} \leq 10^{-2}. \quad (12)$$

The problem (11) in the diffusion boundary layer approximation ($10^{-2} \geq Pe^{-1} = 0$) has the form: namely:

$$\begin{aligned} (1 + FoY^2) \frac{\partial C}{\partial X} &= \frac{\partial^2 C}{\partial Y^2}; \\ X = 0, \quad C = 0; \quad Y = 0, \quad C = 1; \quad Y \rightarrow \infty, \quad C = 0. \end{aligned} \quad (13)$$

The mass transfer rate (J) in the liquid film flow with a length l is the average value of the local mass flux through the face interphase ($y = h_0$). On the other hand this rate can be presented

using the mass transfer coefficient k . As a result

$$J = \frac{D}{l} \int_0^1 \left(\frac{\partial c}{\partial y} \right)_{y=h_0} dx = k(c^* - c_0). \quad (14)$$

In the generalized variables, from (14) the Sherwood number (Sh) is possible to be obtained:

$$Sh = \frac{kl}{D} = -\sqrt{Pe} \int_0^1 \left(\frac{\partial C}{\partial Y} \right)_{Y=0} dX, \quad (15)$$

where $C(X, Y)$ is the solution of (13) [9, 10] developed by a perturbation method [2]:

$$Sh = \sqrt{\frac{6Pe}{\pi}} \left(1 - \frac{Fo}{6} - \frac{19Fo^2}{120} \right). \quad (16)$$

The examined example shows the theoretical techniques, used for the modeling and simulation of the elementary processes in a complex industrial process. The presence of the models of all elementary processes in a complex industrial process does not give a practical opportunity to synthesize its model. The role of modeling and simulation of elementary processes is the theoretical explanation of a number of physical and chemical effects observed experimentally in industrial processes. An illustrative example in this respect is the nonlinear theory of the mass transfer.

3.2. Non-linear mass transfer theory

The theory of the diffusion boundary layer [2] is the basis of modern linear mass transfer theory, where the convection-diffusion equation in (8) is linear, i. e. the velocity does not depend on the concentration. In a number of cases, the experimental results for the mass transfer rate are higher than the predictions of the linear theory [11, 12]. This is due to nonlinear effects, where the mass transfer influences the hydrodynamics and the velocity begin to depend on concentrations. These non-linear effects are related to the induction of secondary flows at the interphase boundaries as a result of interphase mass transfer. Such effects are the effect of large concentration gradients [11], the effect of Marangoni and the effect of Stephan flow [12].

The large concentration gradients create an intensive diffusion flux that have a hydrodynamic character, and a secondary flow is induces, directed at the normal of the interphase boundary and results in an additional convective mass transfer.

The effect of Marangoni is a result of the gradient of the surface tension on the interphase surface, as a result of the surface gradient of the temperature or surface active agents concentration on the liquid-gas (liquid) interphase, and induces a tangential flow. As a result of the continuity of the flow, there appears to be a much lower flow in the direction of the normal of the interphase boundary and consequently an additional convective flow. Because of this, this effect is relatively weak and occurs in motionless or slow moving fluids.

The Stephan's flow is a result of a phase transition liquid-steam at the interphase surface when the volume of the liquid (steam) increases (decreases) a thousand times. As a result, there is a secondary flow, directed to the normal of the interphase boundary, and an additional convective mass transfer.

In the above three cases, an additional hydrodynamic effect appears very often because the secondary currents disturb the hydrodynamic stability of the flows and self-organizing dissipative structures occur, which further accelerate the mass transfer [9]. To these effects can be added the Benar instability [12] in the case of a positive vertical gradient of the density of gases or liquids resulting from concentration or temperature gradients.

The theory of mass transfer allows the construction of the process model if its physical mechanism is known. The model thus obtained allows for the identification of this mechanism, i.e. the determining of the significant physical effects and rejection of the insignificant, using the generalized analysis method [2].

4. Physical mechanism identification

The qualitative analysis of the models permits to be made the physical mechanism identification, using generalized variables [2]. They are dimensionless variables, whereas as the characteristic (inherent) scales are used the maximal or average values of the variables. The introduction of the generalized variables leads to dimensionless model. As a result the unity is the order of magnitude of all functions and their derivatives in the model, i.e. the effects of the physical and chemical phenomena (the contribution of the terms in the model), are determined by the orders of magnitude of the dimensionless parameters in the model. If all model equations are divided by the dimensionless parameter, which has the maximal order of magnitude, all terms in the model equations will be classified in three parts:

1. The parameter is unity or its order of magnitude is unity, i.e. this mathematical operator represents a main physical effect;
2. The parameter's order of magnitude is 10^{-1} , i.e. this mathematical operator represents a small physical effect;
3. The parameter's order of magnitude is $\leq 10^{-2}$, i.e. this mathematical operator represents a very small (negligible) physical effect and has to be neglected, because it is not possible to be measured experimentally.

After the physical mechanism identification the model contains a minimum number of parameters which must be determined experimentally.

5. Parameters identification

In general case, the identification of the parameters in the model is made by the minimization of the least squares function by the inverse identification problem solution [1-3]. The least squares function represents the sum of the squares of the differences between the calculated and the experimental values of the functions in the model and its minimum must be obtained with respect to the parameters in the model. This inverse identification problem is very often incorrect and needs special methods for the solutions [2].

6. Statistical analysis of the model adequacy

The stochastic nature of the errors during the experimental data determination leads to subsequent errors of the model parameters. The model is adequate if the variance of the statistical error of the model does not exceed the variance of the statistical error of the experimental data, i. e. the accuracy of the functions calculation by the model is not less than the accuracy of the function experimental measurement [2, 3].

7. Processes simulation

The process simulation uses the most common numerical methods of applied mathematics to solve model equations. For this purpose, commercial software is usually used. In many cases, however, it is necessary to introduce this software into specialized algorithms [2, 13].

8. Modeling of industrial mass transfer processes in column apparatuses

The diffusion boundary theory is not applicable for the modeling of chemical, absorption, adsorption and catalytic processes in column apparatuses, where the velocity distributions and interphase boundaries are unknown.

The use of the physical approximations of the mechanics of continua for the interphase mass transfer process modeling in industrial column apparatuses is possible if the mass appearance (disappearance) of the reagents on the interphase surfaces of the elementary physical volumes (as a result of the heterogeneous reactions) are replaced by the mass appearance (disappearance) of the reagents in the same elementary physical volumes (as a result of the equivalent homogenous reactions), i.e. the surface mass sources (sinks), caused by absorption, adsorption or catalytic reactions must be replaced with equivalent volume mass sources (sinks). The solution of this problem is related with the creation of new type of convection-diffusion and average-concentration models [13].

The convection-diffusion models permit the qualitative analysis of the processes only, because the velocity distribution in the column is unknown. On this base is possible to be obtained the role of the different physical effect in the process and to reject those processes, whose relative influence is less than 1%, i.e. to be made process mechanism identification.

The average-concentration models are obtained from the convection-diffusion models, where average velocities and concentrations are introduced. The velocity distributions are introduced by the parameters in the model, which must to be determined experimentally.

Conclusions

The theoretical foundations of modeling and simulation of the industrial processes are presented. The first step is the formulation

of the physical mechanism of the industrial process and the construction of a mathematical structure, containing the mathematical operators that quantitatively describe the individual physical effects in this mechanism. The introduction of generalized (dimensionless) variables through characteristic scales permits to be made a quality analysis of the industrial processes. The obtaining of the experimental data and using it to calculate the model parameters by solving a inverse identification problem leads to the final form of the mathematical model. The statistical analysis of the model adequacy leads to the practical applicability of the mathematical model. The presented results are published in 8 monographies (www.iche.bas.bg/Books_BG.htm).

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