Heat and Mass Transfer

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Modeling of Column Apparatus Processes

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*The **mathematical model** of a complex of elementary processes is a **mathematical structure**, where the **mathematical operators** are mathematical descriptions of the **elementary processes**.*

Preface

The complex processes in the column apparatuses have a combination of hydrodynamic processes, convective and diffusive mass (heat) transfer processes, and chemical reactions between the reagents (components of the phases).

The fundamental problem in the column apparatuses modeling is a result of the complicated hydrodynamic behavior of the flows in the columns, and thus, the velocity distributions in the columns are unknown.

The column apparatuses are possible to be modeled, using a new approach on the base of the physical approximations of the mechanics of continua, where the mathematical point is equivalent to a small (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.

The mathematical models of the processes in the column apparatuses, in the physical approximations of the mechanics of continua, will be the mass balances in the phase volumes (phase parts in the elementary volume), between the convective mass transfer (as a result of the fluid motions), the diffusive mass transfer (as a result of the concentration gradients), and the volume mass sources (sinks) (as a result of chemical reactions or interphase mass transfer). In the case of balance between these three effects, the mass transfer processes are stationary or in the opposite case, the processes are non-stationary.

These convection–diffusion-type models permit to be made a qualitative analysis of the processes (models) for to be obtained the main, small, and slight physical effects (mathematical operators), and to be rejected the slight effect (operator). As a result, the process mechanism identification is possible to be made. These models permit to be determinate the mass transfer resistances in the gas and liquid phases and the optimal dispersion system finding in gas absorption (gas–liquid drops or liquid–gas bubbles). The convection–diffusion models are a base of the average concentration models, which allow a quantitative analysis of the processes in column apparatuses.

The convection–diffusion models are possible to be used for qualitative analysis only, because the velocity distribution functions are unknown and cannot be

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obtained. The problem can be avoided by the average concentration models, where the average values of the velocity and concentration over the cross-sectional area of the column are used; that is, the medium elementary volume (in the physical approximations of the mechanics of continua) will be equivalent to a small cylinder with a real radius and a height, which is sufficiently small with respect to the column height and at the same time sufficiently large with respect to the intermolecular distances in the medium.

The convection–diffusion models and average concentration models are used for the qualitative and quantitative analysis of the processes in single phase (simple and complex chemical reactions), two phase (absorption, adsorption, and catalytic processes), and three phase (two-phase absorbent processes and absorption–adsorption processes).

In many cases, the computer modeling of the processes in column apparatuses, on the base of a new approach, using the convection–diffusion-type model and average concentration-type model, does not allow a direct use of the MATLAB. In these cases, it is necessary to create combinations of MATLAB with appropriate algorithms.

Practically, the new type models are characterized by the presence of small parameters at the highest derivatives. As a result, the use of the conventional software for solving of the model differential equations is difficult. This difficulty may be eliminated by an appropriate combination of MATLAB and perturbations method.

In the cases of countercurrent gas–liquid or liquid–liquid processes, the mass transfer process models are presented in two coordinates systems, because in one coordinate system one of the equations has not a solution by reason of the negative equation Laplacian value. A combination of an iterative algorithms and MATLAB must be used for the solutions of the equations set in different coordinate systems.

In the cases of a non-stationary adsorption in gas–solid systems, the presence of mobile (gas) and immobile (solid) phases in the conditions of long-time processes leads to the non-stationary process in the immobile phase and stationary process in the mobile phase, practically. As a result, different coordinate systems must be used in the gas and solid phase models. A combination of a multi-steps algorithms and MATLAB must be used for the solutions of the equations set in different coordinate systems.

The solid fuel combustion in the thermal power plants, which use sulfur-rich fuels, poses the problem of sulfur dioxide removal from the waste gases. This problem is complicated by the fact that it is required to purify huge amounts of gas with low sulfur dioxide concentration. The huge gas amounts need big size apparatuses, which is possible to be decreased if the removal process rate is maximized. The process intensification is realized with a new patent in two-zone column, where the upper zone is physical absorption in a gas–liquid drops system (intensification of the gas phase mass transfer), the lower zone is a physical absorption in liquid–gas bubbles system (intensification of the liquid phase mass transfer), and the chemical reaction takes place in the column tank.

The problem of absorbent regeneration is solved in a new patent, using two steps process—physical absorption of sulfur dioxide by water and adsorption of sulfur dioxide from the water solution by synthetic anionite particles. The adsorbent regeneration is made by ammonium hydroxide solution. The obtained ammonium sulfite solution is used (after reaction with nitric acid) for concentrated sulfur dioxide and ammonium nitrate solution production.

The purification of large amounts of waste gases from combustion plants used countercurrent absorbers, where the gas velocity (as a result and absorbers diameter too) is limited by the rate of the absorbent drops fall in an immobile gas medium. This disadvantage is avoided by a new patent, where cocurrent sulfur dioxide absorption is realized.

The Introduction concerns linear mass transfer theory (model theories, boundary layer theory, and two-phase boundary layers), mass transfer in countercurrent flows (velocity and concentration distribution, and comparison analysis), nonlinear mass transfer (influence on the hydrodynamics, boundary conditions, boundary layer theory, and Marangoni effect), interphase mass transfer resistances (film and boundary layer theories approximations), three-phase mass transfer processes (physical, hydrodynamic and interphase mass transfer models, absorption mechanism, and kinetics).

Part I focuses on the convection–diffusion-type models for qualitative analysis of the column apparatuses processes. In Chap. 2 are presented one-phase chemical processes in column reactors (simple and complex chemical reaction kinetics), approximations of the model (short- and high-columns model, effect of the chemical reaction rate), effect of the radial non-uniformity of the velocity distribution (conversion degree, concentration distribution, influence of the velocity radial non-uniformity shape, scale effect, back mass transfer mechanism), examples (effect of the tangential flow, simultaneous mass and heat transfer processes, circulation zones in column apparatuses, and mass transfer in one-phase countercurrent flow). In Chap. 3 are presented the convection–diffusion-type models of two-phase processes (physical and chemical absorption, physical and chemical adsorption, and catalytic processes in the cases of physical and chemical adsorption mechanism), examples (airlift reactors, airlift photo-bioreactor, and moisture adsorption). In Chap. 4 are presented models of three-phase processes in the cases of two-phase absorbent processes (physical and chemical absorption) and absorption–adsorption processes (physical and chemical adsorption mechanism),

Part II addresses the average concentration-type models for quantitative analysis of the column apparatuses processes. In Chap. 5 are presented the average concentration-type models of the column reactors in the cases of simple and complex chemical reactions (effect of the velocity radial non-uniformity, model parameters identification) and as an example the modeling of a non-isothermal chemical reactor. In Chap. 6 are presented the interphase mass transfer models of the physical and chemical absorption, physical and chemical adsorption, catalytic processes in the cases of physical and chemical adsorption mechanism, and as examples airlift reactor modeling and moisture adsorption modeling.

Part III addresses the calculation problems in the convection–diffusion-type models and average concentration-type models. Chapter 7 presents the perturbation method approach for the solution of the equations in the convection–diffusion models and average concentration models. Chapter 8 presents the solutions of two coordinate systems' problems in the models of the countercurrent absorption processes. Chapter 9 presents the multi-steps modeling algorithms in the case of a long-time non-stationary adsorption process, when the interphase gas–solid mass transfer is stationary.

Part IV concerns the models of the processes, which participate in different patents, related with the waste gas purification from sulfur dioxide in column apparatuses. Chapter 10 presents the modeling of a bizonal absorption apparatus for sulfur dioxide absorption by two-phase absorbent. Chapter 11 presents the processes modeling of an absorption–adsorption method for waste gas purification from sulfur dioxide, where the first step is a physical absorption of sulfur dioxide by water and the second step is a chemical adsorption of sulfur dioxide in the water solution by synthetic anionite. After the sulfur dioxide saturation of the synthetic anionite particles, the adsorbent regeneration is possible to be carried out by water solution of ammonium hydroxide. Chapter 12 presents the processes modeling in a cocurrent apparatus, where the gas velocity is 4–5 times greater than that of the countercurrent apparatus, which are used in the practice.

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