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Simulation of Hydrodynamics and Mass Transfer in Separated Flows Past Packings in Technological Apparatuses

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The intensive researches in hydrodynamics and mass transfer in the technological apparatuses attract today great attention to the study of separated flows for various values of regime parameters and configurations of streamlined packed bodies. The theoretical description of the effect of flow separation on mass transfer, even for simple shape packings, taking into account the vortex interaction, is a non-trivial problem, and it has not yet been completed. The needs of engineering practice force us to look for ways for developing simplified models that adequately reflect the main patterns of the effect of flow separation on the efficiency of mass transfer and for carrying out the optimal calculation of the corresponding equipment.
In this paper, a new approach for calculating the mass transfer coefficient, taking into account the flow separation and its transformation during multistage interaction of gas and droplets has been proposed. Such processes are specially organized, for example, in absorbers. The novelty of the model lies in the fact that it describes the process of mass transfer taking into account the separation in the boundary zone and the redistribution of the velocity profile of the carrier flow when flowing past packed bodies. The theoretical basis of the model is the Reynolds-averaged Navier-Stokes equations, known as dynamic equations for the functions of stream, vorticity, kinetic energy, and local turbulence scale. In the process of flow past packed bodies, two different zones are formed: a multiply connected flow core, which occupies the main area in the contact zone, and a vortex one, generated by separation. Accordingly, modeling and calculation of the mass transfer coefficient were also carried out by different methods, taking into account the distribution of dynamic functions. To ensure sufficient accuracy, stability and convergence of the numerical solution of dynamic equations in the vortex zone, the modified algorithm with a variable step has been developed.
The analysis of the dependences and plots obtained in two directions: verification of the adequacy of the simulation results in terms of the hydrodynamics of separation and the mass transfer coefficient, has been carried out. It is shown that the numerical results are in good agreement with the known experimental data and the previously studied patterns of separated flows. For reliable practical application, this model requires the identification of control parameters for specific physicochemical systems.

1. Introduction

In this paper, the object of research is mass transfer devices with regular plate nozzles (hereinafter referred to as DRPN). In these devices, several periodically arranged nozzles of the same design are installed, around which the stages of gas and liquid contact are organized. In the work (Balabekov, 1985), general patterns of formation, movement and interaction of vortices during the flow of discretely arranged bodies were revealed, on the basis of which a promising group of new heat and mass transfer devices with a regular nozzle of various configurations and perforated plates was created. DRPN devices have found quite wide application for the

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organization of processes of absorption, rectification and purification of gases from harmful impurities. The main feature of breakaway flows during the flow of nozzles is that after the flow separation appears, the flow becomes unsteady and it is necessary to use the appropriate mathematical apparatus of the theory of turbulence for modeling. Currently, the method of direct numerical simulation of large vortices (Large Eddy Simulation, LES) and the method of Reynolds–Averaged Navier-Stokes Equations (Reynolds-Averaged Navier-Stokes Equations, RANS) are used to solve turbulence problems. A comparative analysis of these algorithms and their programs is given in (Malikov and Madaliev, 2021). However, the use of the LES method for calculating wall currents requires either the introduction of additional "empiricism", consisting in parametrization of the layer adjacent to the wall, or the use of grids with a very large number of nodes of the difference grid (Direct Numerical Simulation, DNS) (Cabot W., Moin P. 1999). Therefore, for technical applications, methods based on the solution of the Navier–Stokes equations by the RANS method are more acceptable. On the basis of RANS, the problem of the flow of plates regularly arranged along the axis in DRPN was previously solved (Ismailov et al., 2014). It is established that when a plate with sharp edges flows around (Figure 1), a sudden expansion of the gas flow occurs. In the literature, the number of works devoted to the flow of nozzles in mass transfer devices is not enough. There are only a few detailed numerical studies that thoroughly analyze coherent structures and the destruction of vortices during sudden expansion (Mak H., Balabani S. 2007). Analysis of the results of modeling the hydrodynamics of nozzle flow in turbulent mode in devices with multistage phase interaction (Ismailov, et al., 2022) showed that when calculating mass transfer in different zones of the contact zone, it is necessary to take into account the separation of the flow from the channel and nozzle boundaries. The concentration of droplets in this work is considered small and its effect on the gas flow can be neglected in the first approximation. However, with a higher irrigation density, it is impossible to neglect the effect of droplets on hydrodynamics and the stochastic approach developed in the work (Brener et al., 2017). In this paper, a quantitative assessment of the values of the mass transfer coefficient in different parts of the contact zone of the DRPN with plate nozzles will be made, with respect to the process of evaporation of water droplets by air, taking into account the velocity distribution along the length of the apparatus.

2. Modeling of hydrodynamics in devices with multistage phase interaction

In the paper (Malikov and Madaliev, 2021), a numerical study of a suddenly expanding strongly swirling flow is carried out using the Reynolds stress models SSG/LRR-RSM and EARSM. The conclusions and recommendations of this work are applicable to the problem of gas flow around plates, because in the zones after the flow there is an expansion of the flow. Due to the complexity of the problem, we accept the following simplifications: a) the flow of the gas droplet flow is two-dimensional; b) the closure of the Reynolds equations for turbulence is performed using the Kolmogorov-Prandtl hypothesis; c) the density of liquid irrigation is small. A partial justification for these simplifications are the following considerations: a) the width of the devices with multistage phase interaction currently in operation (devices with multi-stage phase interaction) is large enough and the influence of walls on hydrodynamics in the transverse direction can be neglected; b) in the general formulation, the problem of describing turbulent flow by deterministic methods is currently not solved, at the same time, the use of semi-empirical theories for engineering problem statements gives satisfactory results; c) for the above-mentioned process of evaporation of liquid droplets by air, the irrigation density is L=(0,5÷1) $m^3/(m^2 \cdot hour)$, while the numerical concentration of liquid droplets does not exceed 5% in volume, therefore there is reason to neglect the effect of droplets on the two-phase flow.

2.1 Dynamic functions of the gas flow

The basis of the proposed method is the use of the basic differential equation for the function φ(x,y) (Gosmen A.D., et al., 1972), which is generalized and is equal to one of the functions $\psi(x,y), \omega(x,y), k(x,y), l(x,y),$ fully determining the hydrodynamics in DRPN:

$$a\left[\frac{\partial}{\partial x}\left(\varphi\frac{\partial\psi}{\partial y}\right)-\frac{\partial}{\partial y}\left(\varphi\frac{\partial\psi}{\partial x}\right)\right]-\frac{\partial}{\partial x}\left[b_1\frac{\partial}{\partial x}(c\varphi)\right]-\frac{\partial}{\partial y}\left[b_2\frac{\partial}{\partial y}(c\varphi)\right]+d=0 \tag{1}$$

In a Cartesian two-dimensional system, they coincide with *x,y*. Current function (ψ), vorticity (ω), the kinetic energy of turbulent pulsations (*k*) and the local scale of turbulent pulsations (l), are solutions of the dynamical system Eq.1 (Ismailov B. et al., 2022). To simulate and generate an inhomogeneous gas flow, the cases of flow around a plate located in the middle of a steady-state contact stage and a rotating canna are considered (Figure 1, a and b). The geometry of the channel and nozzles, the input velocity profile is set by boundary and initial conditions.

2.2 Solution domain and finite-difference scheme

To solve the problem (1)-(4) with initial and boundary conditions, a finite difference method was used. The area of numerical solution of the problem is shown in Figure 1. At the initial moment of time, the droplets are considered to be evenly placed at the channel entrance. The further trajectory of the droplets is calculated according to the equation of motion (2).
Figure 2 shows graph of the longitudinal component of the velocity for different distances from the entrance, obtained for the Reynolds number equal to 2500 in the steady-state contact stage in the channel with the plate and in the turning channel. Figure 2 shows that in vortex zones, due to the thickening of the current lines, the maximum values of the longitudinal component of the velocity are almost three times higher than the average outgoing velocity. The longitudinal component of the velocity in the rotating flow (Figure 2) reaches its maximum after the flow around the channel angle.

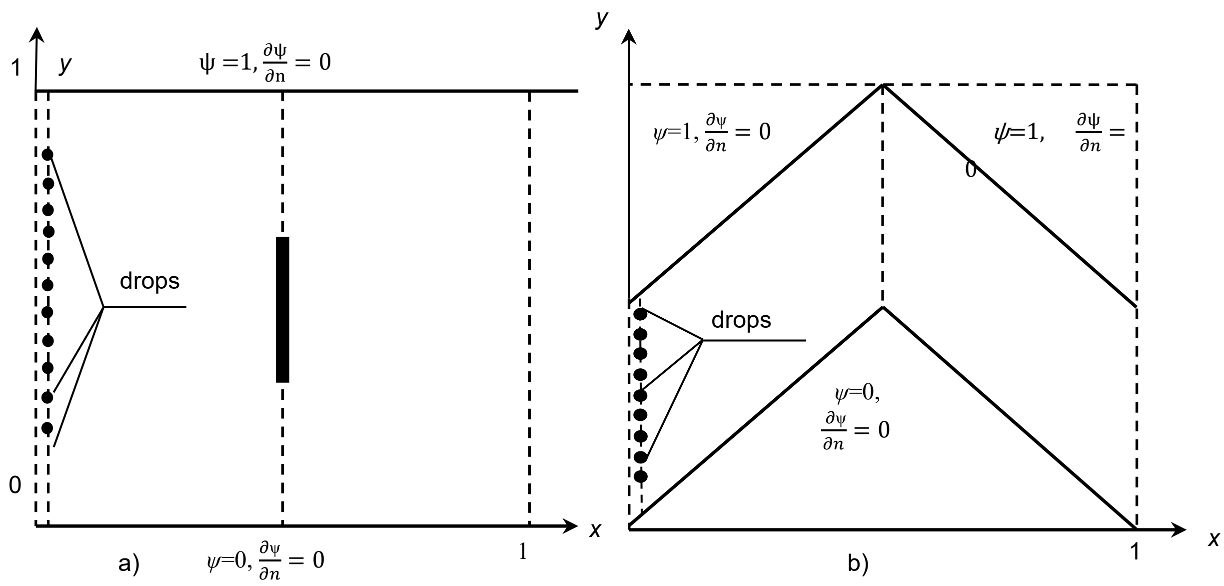

Figure 1. The field of solving the equations of gas motion: a) flow around the plate; b) rotating channel

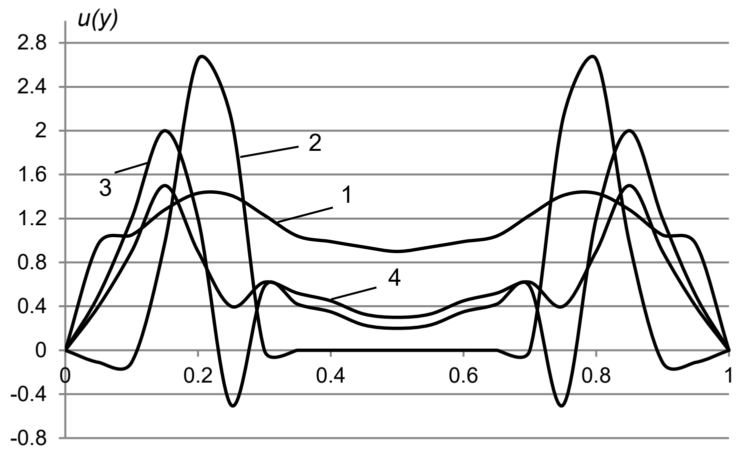

Figure 2. Profiles of the longitudinal velocity of the gas during the flow around the plate, Re = 2500.
x – distance from the entrance to the channel, 1– x = 0,3; 2 – x = 0,5; 3 – x = 0,6; 4 – x = 0,8.

2.3 Modeling and calculation of droplet trajectories

In the two-phase operation mode of DRPN, the liquid flowing down is dispersed by the ascending gas flow into droplets. The differential equation of the motion of a drop is written as (Polyanin et al., 1995):

$$m_d \frac{dW_d}{dt} = \frac{\xi_d}{2} \rho_g f_d W_{rel}^2 \bar{e} + m_d \bar{g} \quad (2)$$

where m_d - drop weight, W_d - drop velocity.

After converting Eq. 2 and reducing it to a dimensionless form, the following system can be written:

$$H_0 \frac{dW_{rel}}{dt} = -kW_{rel}^2 - Fr\, sin\, \alpha_{rel} - P_y\, cos\, \alpha_{rel} - P_x\, sin\, \alpha_{rel} \quad (3)$$

$$H_0 \frac{d\alpha_{rel}}{dt} = -Fr \frac{cos\, \alpha_{rel}}{W_{rel}} + \frac{P_y\, sin\, \alpha_{rel} - P_x\, cos\, \alpha_{rel}}{W_{rel}} + e_y\ \ sin\, \alpha_{rel} - e_y\ \ cos\, \alpha_{rel} \quad (4)$$

$$P_y = \left(\frac{\partial^2 \psi}{\partial x \partial y} \cdot \frac{\partial \psi}{\partial x} - \frac{\partial^2 \psi}{\partial x^2} \cdot \frac{\partial \psi}{\partial y} \right), P_x = \left(-\frac{\partial^2 \psi}{\partial y^2} \cdot \frac{\partial \psi}{\partial x} + \frac{\partial^2 \psi}{\partial x \partial y} \cdot \frac{\partial \psi}{\partial y} \right) \quad (5)$$

$$e_y = \left(\frac{\partial^2 \psi}{\partial x \partial y} cos\, \alpha_{rel} + \frac{\partial^2 \psi}{\partial x^2} sin\, \alpha_{rel} \right), e_x = -\left(\frac{\partial\ \ \psi}{\partial x \partial y} sin\, \alpha_{rel} + \frac{\partial^2 \psi}{\partial x \partial y} cos\, \alpha_{rel} \right) \quad (6)$$

α_{rel} - the angle between the *y* axis and W_{rel}, $k_1 = \frac{3}{4} \xi \frac{\rho \cdot b}{\rho_l \cdot d_d}$

ρ_l - the density of the liquid. In the turbulent mode at Re>10000 it is possible to accept ξ =0.44.

When Eq. 2 is de-dimensioned, homochrony criteria appear $H_0 = \frac{b}{TU_0}$, Froude $Fr = \frac{gb}{U_0^2}$. In Eq.3 and Eq.4 numbers are present P_x, P_y, e_x, e_y which are expressed in terms of derivatives of the current function, which is the solution of the dynamic system for gas.

The algorithm for calculating the trajectory of the droplet movement is as follows:

1. A drop of a certain diameter is considered to be placed at a fixed point. Estimated calculations of the distance from the nozzle showed that the initial position of the formed droplet can be considered the channel zone directly adjacent to the edge of the nozzle.
2. All values $\psi_{i,j}$ и the corresponding values of the derivatives are obtained from the numerical solution of the dynamical system.
3. We find

$$\alpha_{rel}^{(1)} = \alpha_{rel}^{(0)} + \Delta\alpha_{rel}^{(0)} h_\tau, \quad W_{rel}^{(1)} = W_{rel}^{(0)} + \Delta W_{rel}^{(0)} h_\tau \quad (7)$$

h_τ - time step. Calculate the components

$$W_{rel,x}^{(1)} = W_{rel}^{(1)} cos\, \alpha_{rel}^{(1)}, W_{rel,y}^{(1)} = W_{rel,y}^{(1)} sin\, \alpha_{rel}^{(1)} \quad (8)$$

4. We find the components of the velocity of the drop, where

$$W_{k,x}^{(1)} = W_{g,x} + W_{rel,x}^{(1)}, \quad W_{k,y}^{(1)} = W_{g,y} + W_{rel,y}^{(1)} \quad (9)$$

where $W_{g,x} = u_{i,j}, W_{g,y} = v_{i,j}$

5. Calculate the increments of coordinates

$$\Delta x^{(0)} = W_{k,x}^{(1)} \cdot h_\tau, \Delta y^{(0)} = W_{k,y}^{(1)} \cdot h_\tau \quad (10)$$

6. Coordinates of the drop

$$x^{(1)} = x^{(0)} + \Delta x^{(0)}, \quad y^{(1)} = y^{(0)} + \Delta y^{(0)} \quad (11)$$

where $x^{(0)}, y^{(0)}$ - grid coordinates.

7. To continue the calculation, let's check if the drop hits the channel boundaries; If the drop is at a distance less than a spatial step, then the calculation ends.
8. For each calculation of coordinates, the number of time steps is summed up in parallel, which is equal to the time the droplets stay in the contact zone, because the calculation stops when the droplets exit to the next stage of contact or when a drop hits the wall.

For the numerical solution, Eq. 2 is reduced to a system of equations for the relative velocity of the droplet and the angle between the direction of the droplet and the gas. The obtained dynamic characteristics of the inhomogeneous flow in paragraph 2.2 are used to calculate the trajectories of droplets. Figure 3 shows the calculated trajectories of droplets with a diameter of 3 mm in a channel with a plate.

The dotted line shows the isolines of the gas current function. Under the influence of gravity and inhomogeneity of the gas flow in zones 1 and 2, a swarm of particles is formed with an average velocity directed to the upper and lower boundaries, respectively. Zones 1 and 2 can be called zones of a "swarm" of droplets, falling into which large droplets lose their spherical shape and pour into the film. In these zones, the probability of droplet aggregation increases: in zone 1-due to the thickening of the current lines, in zone 2-due to the accumulation of droplets.

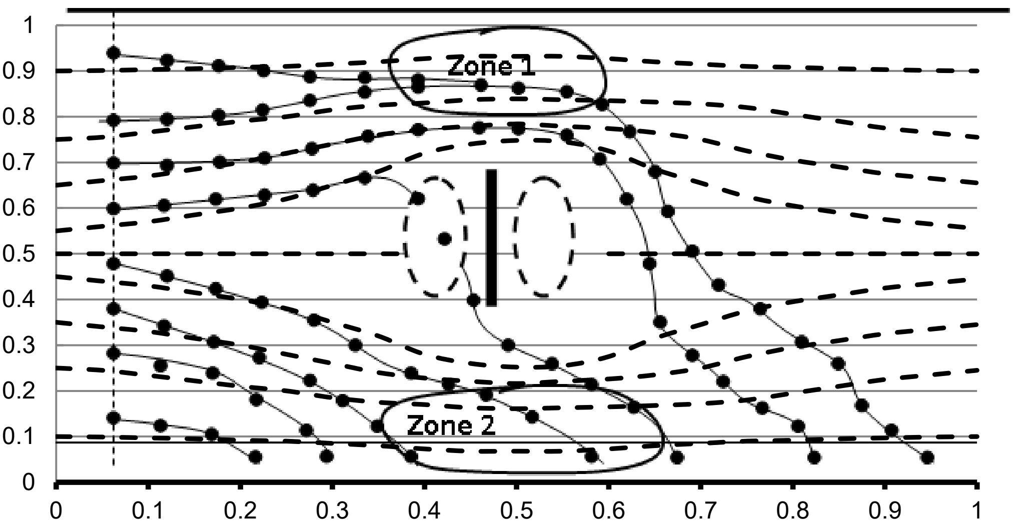

Figure 3. Trajectories of drops in an inhomogeneous gas flow

3. Calculation of the mass transfer coefficient in a channel with plate nozzles

Analysis of the distributions of the gas and droplet velocity components shows that when calculating the mass transfer coefficient in the liquid phase, it is necessary to take into account their sufficiently strong spread. In the literature for a different range of values of the local Reynolds number $\mathrm{Re}_{g,i,j} = \frac{u_{i,j} d\rho}{\mu}$ different formulas are proposed. In the problem under consideration $200 < \mathrm{Re}_{g,i,j} < 10^5$, therefore, the formula is applicable (Polyanin et al., 1995):

$$Sh = Sc^{\frac{1}{3}}\left(0.51\mathrm{Re}_{g,i,j}^{0.5} + 0.0224\mathrm{Re}_{g,i,j}^{0.78}\right) \tag{12}$$

3.1 Results of discussion

Figure 4 shows the dependence of the mass transfer coefficient on the distance from the entrance to the channel of devices with multi-stage phase interaction for the process of evaporation of water droplets by air in the apparatus of devices with multi-stage phase interaction. The values of the Sherwood criterion and the mass transfer coefficient vary greatly depending on the coordinate of the location of the droplets.

The nature of the change in the Sherwood number is qualitatively and quantitatively consistent with the nature of the velocity distribution (Figure 2). This fact must be taken into account when calculating mass transfer in chemical technology devices when the gas flow is inhomogeneous. To increase the size of the zones in which the speed, and accordingly, the mass transfer coefficient takes sufficiently large values, additional devices in the form of guide vanes can be used structurally, with the condition of a small increase in flow resistance.

4. Conclusion

The dynamic characteristics of a turbulent gas flow in a contact device of a mass transfer apparatus with plate nozzles are found by numerical solution of a system of Reynolds equations. The obtained values of the gas velocity in the steady-state section are used to calculate the trajectories of droplets and their residence time in the contact zone. The mass transfer coefficient for the evaporation of water droplets by air is calculated using criterion equations, respectively, for different local values of the Reynolds criterion. The presented approach makes it possible to increase the accuracy of mathematical modeling of mass transfer and hydrodynamics processes in DRPN channels. Thus, by systematic numerical experiment, it is possible to optimize the location and geometry of additional devices in the contact devices of column apparatuses, in order to increase the zones with maximum values of the mass transfer coefficient.

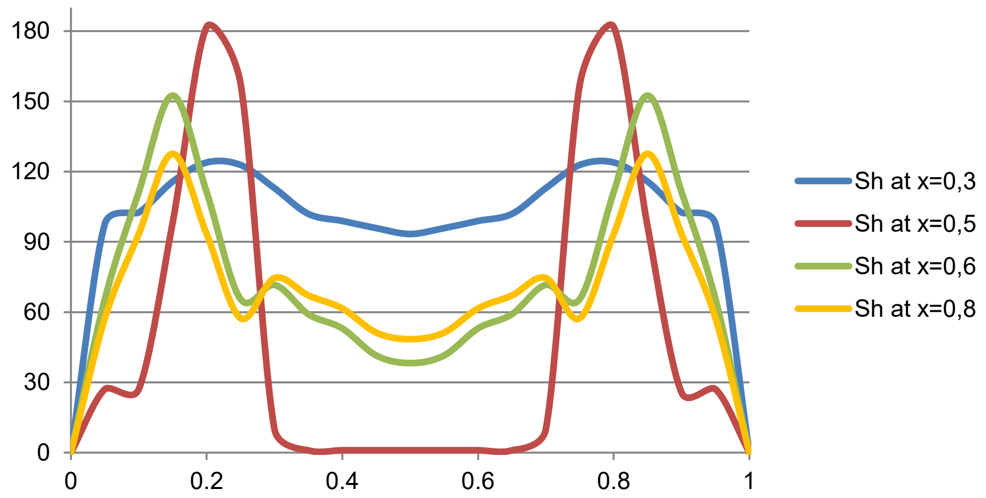

Figure 4 –The dependence of the Sherwood number on the distance from the entrance to the channel: horizontal coordinate – the width of the channel; vertical – the values of the Sherwood number

Nomenclature

a, b_1, b_2, c, d - coefficients determining the type of equations for each dynamic function

f_d - the cross-sectional area of the droplet

$\bar{e}$ - unit direction vector W_{rel}

Re_g - average Reynolds number

$Sh = \beta d_d / D$ - Sherwood criterion

$Sc = \mu / (\rho D)$ - the Schmidt criterion

φ - generalized dynamic function

$\xi_d = f(\mathrm{Re}_g, We)$ - drop resistance coefficient

W_{rel} - relative drop velocity, m/s

$u_{i,j}$ - horizontal component of gas velocity

$v_{i,j}$ - vertical component of gas velocity

We – the Weber criterion

References

Balabekov O.S., 1985, Hydrodynamics, mass transfer and dust collection in countercurrent and cocurrent two-phase drop and film flows in a layer of a movable packing, Dis. Doc. Thesis, Moscow Institute of Chemical Engineering, Moscow.

Brener A., Musabekova L.,Jamankarayeva M., 2017, Stochastic lattice model of aggregation in heterogeneouspolydisperse media, Chemical Engineering Transactions, 60, 79-84. Doi.org/10.3303/CET1760014.

Gosmen A.D., Pan V.M., Ranchel A.K., Spolding D. B., Vol'fshtein M., 1986, Numerical methods for the study of viscous liquid, Mir Space Station, Moscow, USSR.

Cabot W., Moin P., 1999, Approximate wall boundary conditions in the large-eddy simulation of high Reynolds number flow, Flow Turbulence and Combustion, 63, 269-291. Doi.org/10.1023/A:1009958917113.

Ismailov B., Urmatova A., Ismailov Kh., 2014, Modeling and calculation of the trajectory of droplets in a multistage channel mass-transfer apparatus, AIP International Conference on Applied Analysis and Mathematical Modeling (ICAAM-2014), 63-66. Doi.org/10.1063/1.4893805.

Ismailov B., Musabekova L, Umarova Zh, Ismailov, Kh. Arystanbayev K., 2022, Mathematical and computer simulation of particle redistribution and inertial swarming in dispersed systems, Indonesian Journal of Electrical Engineering and Computer Science, 28(2), 909-917. doi.org/10.11591/ijeecs.v28.i2.pp909-917.

Mak H., Balabani S., 2007, Near field characteristics of swirling flow past a sudden expansion, Chemical Engineering Science, 62(23), 6726–6746. Doi.org/10.1016/j.ces.2007.07.009.

Malikov Z.M., Madaliev M.E., 2021, Numerical study of a swirling turbulent flow in a channel with a sudden expansion, Bulletin of Tomsk University, Mathematics and Mechanics, 72, 93-101. Doi.org/10.17223/19988621/72/8

Polyanin A.D., Vyaz'min A.V., 1995, Mass-heat transfer of drops and bubbles with the flow, Theoretical foundations of chemical technology, 29(3), 249-260.