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әл-Фараби атындағы Қазақ ұлттық университетінің

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## ИЗВЕСТИЯ

НАЦИОНАЛЬНОЙ АКАДЕМИИ НАУК  
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## NEWS

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**V.N. Koleskin<sup>1</sup>, A.A. Yunusov<sup>2</sup>, A.A. Yunusova<sup>2</sup>, P.G. Shtern<sup>1</sup>,  
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E-mail: daulet\_ospl@mail.ru

**THE MODELING OF A FLOW IN FLAT AND RADIAL CONTACT UNITS WITH A STILL GRANULAR LAYER. THE SOLVING OF THE PROBLEM IN II DOMAIN (THE COLLECTING MANIFOLD). (PART- 2)**

**Abstract.** Heterogeneous catalytic processes conducted in axial or radial type reactors with a still catalytic layer are some of the most important elements of the chemical technology. The attention of scientists and manufacturers to the investigation and application of these contact units deals with the following advantages: a highly developed surface of a phase separation, a possibility to provide a high flow velocity and hence to decrease sizes and a material consumption, a construction simplicity and a reliability of an exploit. Improving an operation of contact units may be achieved by refining present technologies, catalysts, disperse system structures and by creating new ones. Nevertheless, in some cases large scale hydrodynamic heterogeneities in a working zone of the unit cancel out efforts to increase an efficiency of chemical, heat/mass transfer and other processes. The exploration of reasons of the hydrodynamic heterogeneities formation requires an investigation of liquid and gas motion physics features in granular layers. A practice of a chemical reactors exploitation reveals that technical and economical indicators of an industrial process are as a rule lower than the calculated ones, derived on a stage of the process design. Now it can be considered proven that one of the reasons affecting the reactor output is the heterogeneity of a reagents flow in a granular catalyst layer. The article deals with a mathematical modeling of an incompressible liquid flow in flat and radial contact units with the still granular layer and a creation of numerical realization methods for the model

We propose a cycle of articles dealt with a model of a real reactor that consists of three parts: a distributing manifold, a collecting manifold and a working zone, where the still layer of a granular catalyst is loaded. An input and an output are made with a Z-shaped scheme. We consider processes and their equations in each reactor zone in detail.

**Keywords:** chemical reactor, still granular layer, catalyst, Ergun law, stream function, granular layer resistance factor, Green's function, pressure field, velocity field, layer resistance.

The vast amounts of works are dealt with revealing the equations of an incompressible liquid motion in the still granular layer. These equations are constructed by phenomenological and statistical methods [1-4]. In the first case equations are written down phenomenologically and an interpretation of some parts is conducted using the averaging of a microscopic model [1,2]. The statistical method is based on time, ensemble and space ways of averaging correspondent micro-equations, that describe a continuous one-phase medium motion and the motion of several one-phase media with account for boundary conditions on inter-phase surfaces [3,4]. For deriving the averaging equations the kinetic theory of a disperse media and Vokker-Planck differential equation were applied. As a result of these approaches there were obtained either different modifications of Darcy and Ergun equations or, as in a turbulence theory, non-closed systems of equations that may be closed with account for a structure and physical properties of phases in the mixture [5-7]. This is the main problem in modeling heterogeneous media.

Contact units of a radial type with the still granular material are widely used in technological processes of different industries. A chemical reactor with the still layer of a tableted catalyst that is used in a large-capacity petrochemical industry can be mentioned as an example. One of the reasons that decreases the efficiency of such units is a heterogeneity of a reagents flow in a reactor working zone. It is known that the appearance of heterogeneities in a steam and raw mixture flow is caused by two factors. The first factor is the heterogeneity of the catalyst layer structure, for example, its porosity (or density) that appears during the process of a layer making (in filling the unit) [8-10] and during the further operation as a result of packing by gravity, vibration, breaking catalyst granules and so on. The second one is a bad choice of a ratio between geometrical and hydraulic parameters of a unit during its design.

It is considered that the heterogeneity of the reagents flow in the reactor working zone sufficiently influences process indicators only if a chemical reaction takes place either near the catalyst surface or on it. Indeed, at these conditions the velocity of reacting products directly defines the time of a contact with the catalyst. Main characteristic parameters of the reaction depend on this time. If the reaction takes place inside a porous space of catalyst granules then the contact time is defined by a diffusive reagents velocity and does not depend on a flow velocity near the granule. In the case it is assumed that the flow heterogeneity does not influence the chemical reaction kinetics.

Indeed that is not so. The majority of practically using reactions are accompanied by heat consumption or emission, so they are endothermic or exothermic. Hence if the reaction takes place in an interdiffusive area then some heat should be brought in or out, because the efficiency of the reaction often depends upon a temperature. To hold the specified temperature regime of the catalyst layer a neutral heat carrier, for example an overheated steam, is added to source reactants. It is well known that the flow heterogeneity of such steam-raw mixture causes an inhomogeneous temperature field and therefore leads to an appearance of overcooled or overheated parts in the catalyst layer. In addition to decreasing the output of a target product that results in sintering the catalyst or losing its catalytic properties.

Heterogeneities in the catalyst layer structure may be removed by using special ways of loading [11-16] or by an application a modular catalyst, where it is possible. By now these ways of loading and the technology of the catalyst module production have been already invented and continue to be developed. The flow nonuniformity that is caused by the reactor construction may be investigated and removed on the base of hydroaerodynamic calculations which allow to define the velocity and pressure fields in the unit in dependence on its geometrical and hydraulic parameters.

Let us consider the calculating of flow parameters in the collecting manifold on a boundary between *II* and *III* domains. Let the outside collector consists of two sub-domains *A* and *B* (fig. 1). The *B* domain is a semi-restricted pipe of  $R_2$  radius. The *A* domain is a semi-restricted coaxial domain with an outer radius  $R_{an}$  and the inner radius  $R_2$ . A boundary between a working zone and the outer collector is denoted as  $\Gamma_2$  and the boundary between *A* and *B* is denoted as  $\Gamma_3$ . Deviations of a real geometry from the selected scheme cannot lead to a significant change of the velocity flow near the  $\Gamma_2$  boundary at distances much more than the collector width  $R_{an} - R_2$ .

The problem of finding the flow in the collecting manifold can be divided into three parts:

- 1) the finding of the flow in the *A* domain upon the velocity normal component specified at  $\Gamma_2$  and  $\Gamma_3$  boundaries;
- 2) the finding of the flow in the *B* domain upon the velocity normal component specified at  $\Gamma_3$  boundary;
- 3) the finding of the velocity normal component at  $\Gamma_3$  upon a condition of the velocity tangential component continuity at the boundary.

The solution of the problem 2 is accomplished like the solution of the problem for the distribution manifold since the *B* domain is the semi-restricted pipe, too. To solve the problem 3 it is necessary to parameterize the velocity normal component  $v_r$  with  $N$  parameters  $C_n$ :

$$v_r(z)|_{\Gamma_3} = \sum_{n=1}^N C_n \varphi_n(z), \quad (1)$$

where  $\varphi_n(z)$  are some specified functions. The solutions of 1 and 2 problems allow find the velocity tangential components  $v_z^{(AB)}$  in *A* and *B* domains that will be linear functions of  $C_n$  due to a linearity of the task:

$$v_z^{(A)}|_{\Gamma_3} = \varphi_0^{(A)}(z) + \sum_{n=1}^N C_n \varphi_n^{(A)}(z),$$

$$v_z^{(B)}|_{\Gamma_3} = \sum_{n=1}^N C_n \varphi_n^{(B)}(z). \quad (2)$$

A free term  $\varphi_0^{(A)}$  is related to a flow that enters in the  $A$  domain through  $\Gamma_2$  boundary. Equating the tangential components  $v_z^{(A)}$  and  $v_z^{(B)}$  at some  $N$  points of  $\Gamma_2$  boundary, we obtain the system of linear equations for the determination of the velocity normal component parameters. A numerical solution of a linear equation system is a well-known task and is conducted via standard computer programs that do not need many computing time. The most consuming part of solving the problem of finding the flow in the outer collector is the problem 1, i.e. the determination of the flow in the  $A$  domain.

### Green's function of a coaxial pipe

To solve the problem of finding the flow of the incompressible liquid in a semi-restricted coaxial domain with a porous inner boundary Green's functions were used [17]. Using modified Green's and Hankel's functions [18-21] and expressing the solution as a Fourier integral we have obtained:

$$v(r, z) = \int \left( v_1^{(R)}(r, z) \Phi_1^{(R)} v_2^{(R)}(r, z) \Phi_2^{(R)} \right) dk \quad (3)$$

$\Phi_1^{(R)}$  and  $\Phi_2^{(R)}$  coefficients are defined from the conditions that the normal component of the velocity equals to zero on the outer boundary at  $r = R_{an}$  and  $v_r(R_2, z)$  equals to the specified  $v_n(z)$  function on the inner boundary.

After transformations the desired expression for the velocity looks like:

$$v(r, z) = \int_{-\infty}^{\infty} G(r, z - \tilde{z}) \cdot v_n(\tilde{z}) d\tilde{z}, \quad (4)$$

where  $G(r, z) \equiv \{G_r(r, z), G_z(r, z)\}$  is Green's function of an unbounded coaxial domain.

Since Green's function must be real a real part of the integrand in the formula for  $G_r$  is an even function of  $k$ , and an imaginary one is odd while in the formula for  $G_z$  this is backwards: the real part is odd and the imaginary part is even. At this reason we rewrite expressions for Green's function without imaginary values:

$$G_r(r, z) = \frac{1}{p} \int_0^{\infty} \frac{J_1(kR_{an})K_1(kr) - J_1(kr)K_1(kR_{an})}{J_1(kR_{an})K_0(kR_2) - J_0(kR_2)K_1(kR_{an})} \cdot \cos kz dk,$$

$$G_z(r, z) = \frac{1}{p} \int_0^{\infty} \frac{J_1(kR_{an})K_0(kr) - J_0(kr)K_1(kR_{an})}{J_1(kR_{an})K_1(kR_2) - J_1(kR_2)K_1(kR_{an})} \cdot \sin kz dk. \quad (5)$$

To find the flow in the semi-restricted domain let us extend it to the unbounded one by a reflection relative to a  $z = 0$  plane.

In this unbounded domain the solution is defined by (4), where  $v_z(z)$  is a symmetrical function of  $z$ . Hence,

$$v(r, z) = \int_{-\infty}^0 G(r, z - \tilde{z}) v_n(\tilde{z}) d\tilde{z} + \int_0^{\infty} G(r, z - \tilde{z}) v_n(\tilde{z}) d\tilde{z},$$

Replacing  $\tilde{z}$  by  $-\tilde{z}$  we obtain that in the  $\tilde{z} < 0$  domain the solution looks like

$$v(r, z) = \int_{-\infty}^0 \{G(r, z - \tilde{z}) + G(r, z + \tilde{z})\} \cdot v_n(\tilde{z}) d\tilde{z} \quad (6)$$

Equations (5) and (6) are the solutions of the problem of finding the flow in a semi-restricted coaxial pipe.

The analytic expression (5) for Green's function is valid in any coaxial domain. But a procedure of the numerical calculating of integrals (5) for a narrow coaxial domain has some features. They deal with the fact that the geometry of a narrow domain is characterized by two sharply different sizes:  $R_2$  radius and a width  $\Delta = R_{an} - R_2$  and  $\Delta \ll R_2$ . To calculate integrals (5) with a proper accuracy we should choose the upper limit of the integration  $\tilde{k} \gg 1/\Delta$  (for example,  $\tilde{k} = 10/\Delta$ ).

The integration step  $\Delta k$  should be so tiny that  $\Delta k \ll 1/R_2$  (for example,  $\Delta k = 1/10R_2$ ). Then a net will consist of  $N = \frac{\tilde{k}}{\Delta k} = \frac{100R_2}{\Delta}$  points and  $N = 10^3$  at  $\frac{R_2}{\Delta} = 10$ . Since the integral should be calculated at

different  $r$  and  $z$ , in each net point the special functions must be calculated and the time for finding Green's functions becomes extremely large. Moreover an argument value of special functions  $\tilde{k}R_2$  reaches  $10R_2/\Delta \approx 100$ , and as special functions grow exponentially their values exceed maximum allowed ones and integrals (5) cannot be calculated at all.

To avoid these difficulties the integration domain  $[0; +\infty]$  should be divided into three parts: from zero to  $\tilde{k}_1$ , from  $\tilde{k}_1$  to  $\tilde{k}_2$  and from  $\tilde{k}_2$  to the infinity. The full integral will be a sum of integrals over these domains

$$G = G^{(1)} + G^{(2)} + G^{(3)} \quad (7)$$

The  $\tilde{k}_1$  value is chosen so that  $\tilde{k}_1 \gg R_2^{-1}$  (but  $\tilde{k}_1$  may be less than  $\Delta^{-1}$ ). For calculating  $G^{(1)}$  we will use the following:

$$G_r^{(1)}(r, z) = \frac{1}{p} \int_0^{R_1} \frac{J_1(kR_{an})K_1(kr) - J_1(kr)K_1(kR_{an})}{J_1(kR_{an})K_0(kR_2) - J_0(kR_2)K_1(kR_{an})} \cdot \cos kz dk, \quad (8)$$

$$G_z^{(1)}(r, z) = \frac{1}{p} \int_0^\infty \frac{J_1(kR_{an})K_0(kr) - J_0(kr)K_1(kR_{an})}{J_1(kR_{an})K_1(kR_2) - J_1(kR_2)K_1(kR_{an})} \cdot \sin kz dk.$$

At  $k \rightarrow 0$  terms under integrals contain an indeterminate form  $0/0$  that should be evaluated analytically. Since

$$z \rightarrow 0, K_0(z) \rightarrow \ln z, K_1(z) \rightarrow z^{-1}, j_0(z) \rightarrow 1, j_1(z) \rightarrow \frac{1}{2} z,$$

then at  $k = 0$  the term under the integral for  $G_r^{(1)}$  equals to:

$$G_r^{(1)} = R_2(R_{an}^2 - r^2)[r(R_{an}^2 - R_2^2)]^{-1},$$

and for  $G_z^{(1)}$  equals to:

$$G_z^{(1)} = (-2zR_2)(R_{an}^2 - R_2^2)^{-1}.$$

At  $k > \tilde{k}_1$  Bessel functions are much more than 1 and asymptotic expansions are valid [19]:

$$J_0(z)|_{z \rightarrow \infty} \rightarrow \frac{1}{\sqrt{2pz}} \cdot e^z \left(1 + \frac{1}{8}z^{-1} + \dots\right),$$

$$J_1(z)|_{z \rightarrow \infty} \rightarrow \frac{1}{\sqrt{2pz}} \cdot e^z \left(1 - \frac{3}{8}z^{-1} + \dots\right), \quad (9)$$

$$K_0(z)|_{z \rightarrow \infty} \rightarrow \sqrt{\frac{p}{2z}} \cdot e^{-z} \left(1 - \frac{1}{8}z^{-1} + \dots\right),$$

$$K_1(z)|_{z \rightarrow \infty} \rightarrow \sqrt{\frac{p}{2z}} \cdot e^{-z} \left(1 + \frac{3}{8}z^{-1} + \dots\right). \quad (10)$$

Correspondingly the expression for  $G^{(2)}$  will be

$$G_r^{(2)} = \frac{1}{p} \sqrt{\frac{R_2}{r}} \int_{\tilde{k}_1}^{\tilde{k}_2} \left\{ e^{k(R_{an}-r)} \cdot \left[1 - \frac{3}{8k} \left(\frac{1}{R_{an}} - \frac{1}{r}\right)\right] - e^{-k(R_{an}-r)} \cdot \left[1 + \frac{3}{8k} \left(\frac{1}{R_{an}} - \frac{1}{r}\right)\right] \right\} D^{-1} \cdot \cos kz dk \quad (11)$$

$$G_z^{(2)} = -\frac{1}{p} \sqrt{\frac{R_2}{r}} \int_{\tilde{k}_1}^{\tilde{k}_2} \left\{ e^{k(R_{an}-r)} \cdot \left[1 - \frac{3}{8k} \left(\frac{1}{R_{an}} + \frac{1}{r}\right)\right] + e^{-k(R_{an}-r)} \cdot \left[1 + \frac{3}{8k} \left(\frac{1}{R_{an}} + \frac{1}{r}\right)\right] \right\} D^{-1} \cdot \sin kz dk \quad (12)$$



where

$$D = e^{k(R_{an}-R_1)} \cdot \left[ 1 - \frac{3}{8k} \left( \frac{1}{R_{an}} - \frac{1}{R_2} \right) \right] - e^{-k(R_{an}+R_2)} \cdot \left[ 1 + \frac{3}{8k} \left( \frac{1}{R_{an}} - \frac{1}{R_2} \right) \right]$$

Taking into account two terms of asymptotic expansions is necessary so that even at  $\eta = \tilde{k}_1 R_1 \approx 10$  the accuracy was about  $(\tilde{k}_1 R_2)^{-2} \approx 1\%$ .

Green's function is a flow that forms in the infinite coaxial domain at  $v_n(z)$  equaled to  $\delta(z)$  — the Dirac delta function, that is if the finite liquid flow equaled to  $2\pi R_2$  enters the domain through an infinitely narrow ring slot set at  $z = 0$ . It is obvious that at moving away from the slot the flow should level off and  $r$  component of the velocity must turn into zero and  $z$  component tends to a constant. It is explicitly from the physics and numerical calculations confirm that this aligning should occur at distances comparable with the width of the domain, i.e. at  $|z| \sim \Delta$ . Therefore the only characteristic size —  $\Delta$  — enters the integral (12) and in its calculating the net should be chosen so that  $\Delta k \ll \Delta$  (but  $\Delta k$  may be more than  $1/R_2$ ).

The necessity of the third integration domain from  $R_{an}$  to  $\infty$  deals with the fact that at  $r \rightarrow R_2$  the terms under integral approach zero very slowly and at  $r = R_2$  they don't reach zero at all and become oscillating. Thus a numerical determination of these integrals is not possible and it is necessary to make an analytic evaluation. This is not difficult if  $\tilde{k}_2 \gg 1/\Delta$ . Then the number of terms with  $e^{-k\Delta}$  is much less than the number of terms with  $e^{-k\Delta}$  and may be neglected. After that the analytic integration is made by standard techniques. We have:

$$G_r^{(3)} = \frac{1}{p} \left\{ \sqrt{\frac{R_2}{r}} \cdot e^{-\tilde{k}_2(r-R_2)} \cdot \frac{(r-R_2)\cos\tilde{k}_2 z - z\sin\tilde{k}_2 z}{(r-R)^2 + z^2} - \sqrt{\frac{rR_2}{R_{an}^2}} \cdot e^{-\tilde{k}_2(2R_{an}-R_2-r)} \cdot \frac{(2R_{an}-R_2-r)\cos\tilde{k}_2 z - z\sin\tilde{k}_2 z}{(2R_{an}-R_2-r)^2} \right\} \quad (13)$$

$$G_r^{(3)} = \frac{1}{p} \left\{ \sqrt{\frac{R_2}{r}} \cdot e^{-\tilde{k}_2(r-R_2)} \cdot \frac{(r-R_2)\sin\tilde{k}_2 z + z\cos\tilde{k}_2 z}{(r-R)^2 + z^2} + \sqrt{\frac{rR_2}{R_{an}^2}} \cdot e^{-\tilde{k}_2(2R_{an}-R_2-r)} \cdot \frac{(2R_{an}-R_2-r)\sin\tilde{k}_2 z + z\cos\tilde{k}_2 z}{(2R_{an}-R_2-r)^2} \right\}$$

Note that  $G^{(3)}$  contains all singularities that appear in the flow at  $r \rightarrow R_2$  and  $z \rightarrow 0$ . Denoting  $r \rightarrow R_2 = \varepsilon > 0$  we have that at  $z \rightarrow 0$ ,  $\varepsilon \rightarrow 0$ :

$$G_r(r, z) \rightarrow \frac{1}{p} \cdot \frac{e}{e^2 + z^2} \Big|_{\varepsilon \rightarrow 0} \rightarrow \mathcal{A}(z) \quad (14)$$

$$G_r(r, z) \rightarrow \frac{1}{p} \cdot \frac{z}{e^2 + z^2} \Big|_{\varepsilon \rightarrow 0} \rightarrow \frac{1}{pz}$$

The numerical finding of Green's function was carried out for the outer manifold of Nizhnekamsk reactor for the styrene production. Results are presented in the fig. 2. One of the qualitative conclusions is that at  $z = R_{an} - R_2 = \Delta$  the flow may be considered as homogeneous with 10% accuracy that is the influence of a disturbance on the manifold boundary spreads out the distance about  $\Delta$ .

Let us analyze the spreading of the flow leaving the collecting manifold. Consider that the normal component of the velocity has rectangular profile at the boundary between the working zone and the outer manifold ( $\Gamma_2$  boundary, fig. 1).

A parameterization of the normal component of the velocity on the boundary  $\Gamma_3$  is carried out under the following reasons:

$$v_r(z)|_{\Gamma_3} = e^{-z/l_1}(a_0 + a_1z + a_2z^2 + \dots) + e^{-z/l_2}(b_0 + b_1z + b_2z^2 + \dots), \quad (15)$$

where  $\Gamma_3$  is the boundary between  $A$  and  $B$  domains;  $l_1$  and  $l_2$  are the characteristic sizes of the task ( $l_1 < l_2$ ),  $z \in (0; \infty)$ . Parameters  $a_0, a_1, \dots, b_0, b_1, \dots$  are defined under the condition of the continuity of the tangential component on the boundary  $\Gamma_3$  and the conservation of the full flow. The last condition is the following:

$$\int_{\Gamma_3} v_r dz = -R_2 R_{\text{ан}}^{-2} \quad (16)$$

or taking into account that integrals from  $e^{-z/l_{1,2}} \cdot z^n$  are taken in explicit form

$$l_1 b_0 - 1! l_1^2 b_1 + 2! l_1^3 a_2 - 3! l_1^4 a_3 + \dots + l_2 b_0 - 1! l_2^2 b_1 + 2! l_2^3 b_2 - \dots = -R_2 R_{\text{ан}}^{-2}. \quad (17)$$

The eq. (15) provides the continuity of the tangential component at  $x \rightarrow \infty$ .

At numerical finding parameters of normal component of the velocity on the boundary we used requirements of the continuity of the normal component at  $z = 0$  and  $z = \Delta/2$  in addition to eq. (15). Under these three conditions parameters  $a_0, a_1$  and  $b_0$  were obtained by solving the system of linear equations.

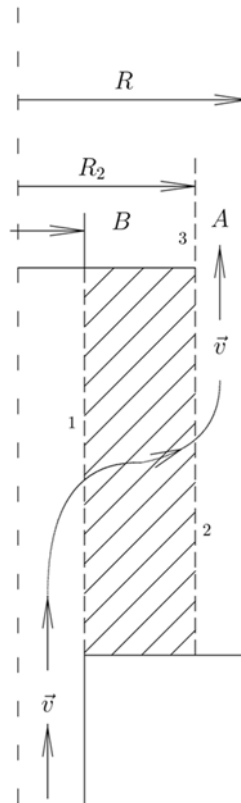


Figure 1 - The outer manifold

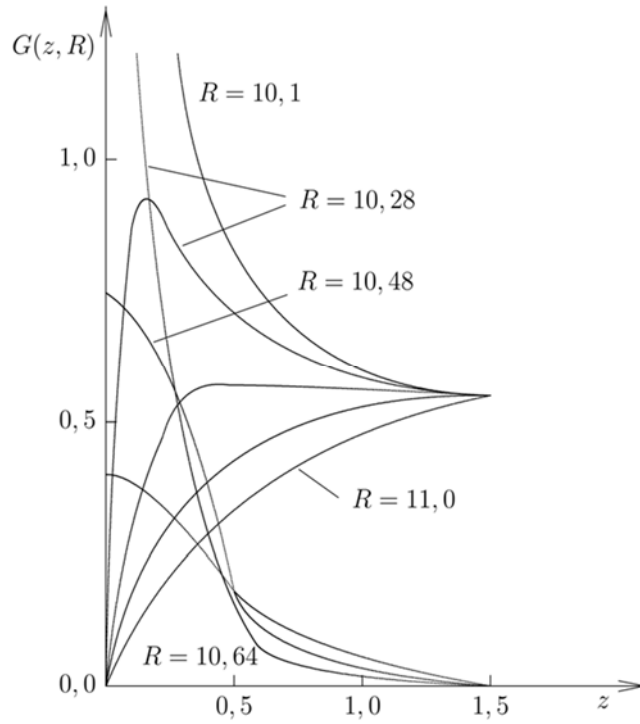


Figure 2 - The universal Green's function for various  $R$  values

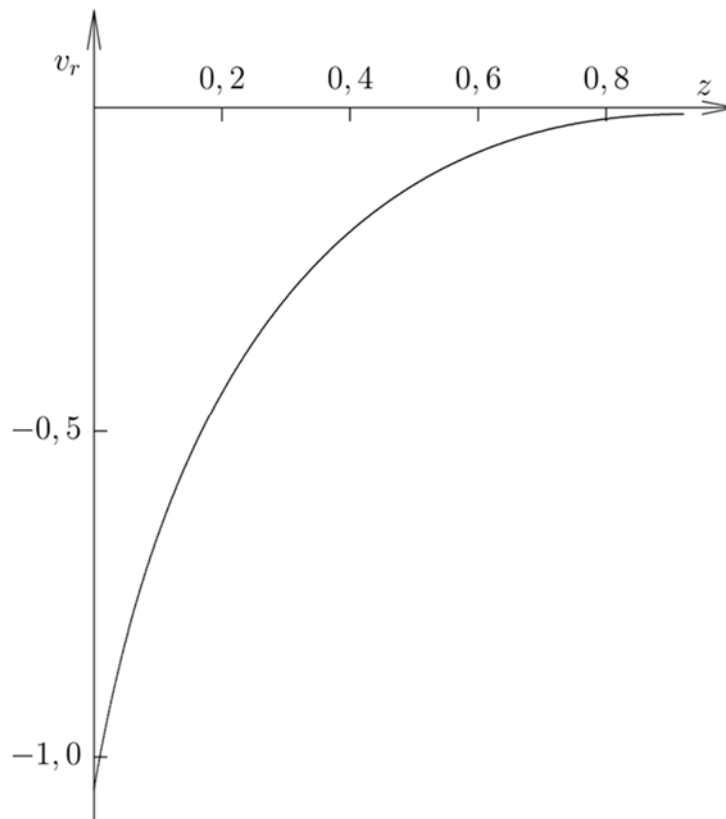


Figure 3 - The profile of the normal component of the relative velocity

Dimensionless coefficients  $c_1 = \frac{l_1}{\Delta}$  and  $c_2 = \frac{l_2}{R_2}$  were determined under the condition that the parameterization provides the continuity of the tangential component of the velocity in average on the boundary the best way. We made a functional equaled to the average square of a jump of the tangential component of the velocity on the boundary

$$F(c_1, c_2) = \int_{\Gamma_3} (v_z^A - v_z^B)^2 dz \quad (18)$$

and parameters  $c_1$  and  $c_2$  were defined under the condition of the  $F$  functional minimum. It results in

$$c_1 = 0,69 \text{ and } c_2 = 0,31 \quad (19)$$

Parameters  $a_0$ ,  $a_1$  and  $b_0$  were

$$a_0 = -0,70, a_1 = -2,79 \text{ and } b_0 = -0,53 \quad (20)$$

(a normalization of these coefficients is determined by an amplitude of the normal component of the velocity on the boundary  $\Gamma_2$  and may be considered arbitrary). At these parameter values the calculation error of the tangential component was about 5%. A profile of the normal component of the velocity is shown in the fig. 3. The fig. 3 shows that the profile of the normal component of the velocity on the boundary  $\Gamma_3$  (i.e. in the output hole of the outer manifold) is mainly determined by the characterized size  $\Delta$  and therefore the disturbance related to a sudden widening has the size of the same order. The part of the profile that has the characterized size  $R_2$  has an amplitude less or about 5%, if exists at all.

**В.Н. Колескин<sup>1</sup>, А.А. Юнусов<sup>2</sup>, А.А. Юнусова<sup>2</sup>, П.Г. Штерн<sup>1</sup>,  
А.В. Лукьянова<sup>1</sup>, М.А. Амандыков<sup>2</sup>, Д.К. Жумадуллаев<sup>3</sup>**

<sup>1</sup>ФБГОУ «Ресей ЖБФМ К.Д.Ушинский атындағы Ярославль мемлекеттік педагогикалық университеті», Ярославль, Ресей;

<sup>2</sup>Қазақстан инженерлі-педагогикалық Халықтар достығы университеті, Шымкент, Қазақстан;

<sup>3</sup>М.Әуезов атындағы Оңтүстік Қазақстан мемлекеттік университеті, Шымкент, Қазақстан

## **АҒЫНДЫ ҚОЗҒАЛМАЙТЫН ТҮЙІРШІКТІ ҚАБАТЫ БАР ЖАЗЫҚ ЖӘНЕ РАДИАЛДЫ БАЙЛАНЫС АППАРАТТАРДА МОДЕЛЬДЕУ. II САЛАДАҒЫ ЕСЕПТЕРДІ ШЕШУ(ЖИНАУШЫ КОЛЛЕКТОР). (2 бөлім)**

**Аннотация.** Химиялық технологияның маңызды элементтерінің бірі катализатордың қозғалмайтын қабаты бар аксиальді немесе радиалды түрдегі реакторларда іске асырылатын гетерогенді каталитикалық процестер болып табылады. Ғалымдар мен өндірушілердің назарына осындай байланыс құрылғыларын зерттеу мен қолдануға бірқатар артықшылықтар себеп болған: фазалар бөлімінің жоғары дамыған беті, ағындардың жоғары жылдамдықтарын қамтамасыз ету мүмкіндігі, демек, габариттер мен материал сыйымдылығын азайту, конструкцияның қарапайымдылығы мепайдаланудағы сенімділік. Байланыс аппараттарының жұмысын жақсартуға қолданыстағы технологияларды жетілдіру және жаңа технологияларды, катализаторлар мен дисперсиялық жүйелердің құрылымдарын құру есебінен қол жеткізілуі мүмкін. Алайда, бірқатар жағдайларда аппараттың жұмыс аймағында ірі масштабты гидродинамикалық біртекті еместіктердің болуы химиялық, жылу-масса алмасу және басқа да процестердің тиімділігін арттыру бойынша іс-әрекетті жокқа шығарады. Гидродинамикалық біртекті емес құбылыстардың пайда болу себептерін анықтау түйіршікті қабаттарда сұйықтық пен газдың қозғалыс физикасының ерекшеліктерін зерттеуді талап етеді. Химиялық реакторларды пайдалану тәжірибесі өнеркәсіптік процестің техникалық-экономикалық көрсеткіштері, әдетте, осы процесті жобалау сатысында алынған есептік мәндерден төмен екендігін куәландырады. Қазіргі уақытта реактордың өнімділігіне әсер ететін себептердің бірі түйіршікті катализатордың қабатындағы реагенттер ағынының біртекті еместілігі болып табылатыны дәлелденген деп санауға болады. Жұмыс қозғалмайтын түйіршікті қабаты бар жазық және радиалды контактілі аппараттарда қысылмайтын сұйықтықтың ағынын математикалық модельдеуге және осы модельді сандық іске асыру әдістерін құруға арналған. Үш бөліктен тұратын нақты реактордың моделі бойынша жұмыс циклі ұсынылды: таратушы коллектор, жинайтын коллектор және түйіршікті катализатордың қозғалмайтын қабаты жүктелетін жұмыс аймағы. Газ ағынын модельге енгізу және шығару Z - бейнелі схема

бойынша жүзеге асырылады. Реактордың әрбір аймағындағы процестер мен олардың сипаттайтын теңдеулерді егжей-тегжейлі қарастырайық.

**Түйін сөздер:** химиялық реактор, қозғалмайтын түйіршікті қабат, катализатор, Эрган заңы, ток функциясы, түйіршікті ортаның кедергі факторы, Грин функциясы, қысым өрісі, жылдамдық өрісі, қабат кедергісі.

**В.Н. Колескин<sup>1</sup>, А.А. Юнусов<sup>2</sup>, А.А. Юнусова<sup>2</sup>, П.Г. Штерн<sup>1</sup>,  
А.В. Лукьянова<sup>1</sup>, М.А. Амандыков<sup>2</sup>, Д.К. Жумадуллаев<sup>3</sup>**

<sup>1</sup>ФБГОУ «Ярославский государственный педагогический университет  
им. К.Д.Ушинского Минвышобрнауки России» Ярославль, Россия;

<sup>2</sup>Университет Дружбы народов имени академика А.Куатбекова, Шымкент, Казахстан;

<sup>3</sup>Южно-Казахстанский государственный университет им.М.Ауэзова, Шымкент, Казахстан

### **МОДЕЛИРОВАНИЕ ТЕЧЕНИЯ В ПЛОСКИХ И РАДИАЛЬНЫХ КОНТАКТНЫХ АППАРАТАХ С НЕПОДВИЖНЫМ ЗЕРНИСТЫМ СЛОЕМ. РЕШЕНИЕ ЗАДАЧИ В ОБЛАСТИ II (СОБИРАЮЩИЙ КОЛЛЕКТОР). (Часть 2)**

**Аннотация.** Одними из важнейших элементов химической технологии являются гетерогенные каталитические процессы, реализуемые в реакторах аксиального или радиального типа с неподвижным слоем катализатора. Вниманию учёных и производителей к исследованию и применению таких контактных устройств обусловлено рядом преимуществ: высокоразвитой поверхностью раздела фаз, возможностью обеспечения высоких скоростей потоков и, следовательно, уменьшения габаритов и материалоемкости, простотой конструкции и надёжностью в эксплуатации. Улучшение работы контактных аппаратов может быть достигнуто за счёт усовершенствования существующих и создания новых технологий, катализаторов и структур дисперсных систем. Однако, в ряде случаев наличие крупномасштабных гидродинамических неоднородностей в рабочей зоне аппарата сводит на нет усилия по повышению эффективности химических, тепло-массообменных и других процессов. Выяснение причин возникновения гидродинамических неоднородностей требует изучения особенностей физики движения жидкости и газа в зернистых слоях. Опыт эксплуатации химических реакторов свидетельствует о том, что технико-экономические показатели промышленного процесса как правило ниже расчётных значений, полученных на стадии проектирования этого процесса. В настоящее время можно считать доказанным, что одной из причин, влияющих на производительность реактора, является неоднородность потока реагентов в слое зернистого катализатора. Работа посвящена математическому моделированию течения несжимаемой жидкости в плоских и радиальных контактных аппаратах с неподвижным зернистым слоем и построению методов численной реализации этой модели. Предложен цикл работ по модели реального реактора, состоящего из трех частей: раздающего коллектора, собирающего коллектор и рабочей зоны в которую загружается неподвижный слой зернистого катализатора. Ввод и вывод газового потока в модели осуществлен по Z-образной схеме. Рассмотрим подробно процессы и описываемые их уравнения в каждой зоне реактора.

**Ключевые слова:** химический реактор, неподвижный зернистый слой, катализатор, закон Эргана, функция тока, фактор сопротивления зернистой среды, функция Грина, поле давлений, поле скоростей, сопротивление слоя.

#### **Information about authors:**

Yunusov Anarbay Aulbekovich, Candidate of Physical and Mathematical Sciences, assistant professor, Kazakhstan Engineering and Pedagogical University of Peoples' Friendship, Shymkent, Kazakhstan, e-mail: [yunusov1951@mail.ru](mailto:yunusov1951@mail.ru), <https://orcid.org/0000-0002-0647-6558>;

Yunusova Altynai Anarbaevna, Candidate of Technical Sciences, assistant professor, Kazakhstan Engineering and Pedagogical University of Peoples' Friendship, Shymkent, Kazakhstan, e-mail: [altyn\\_79@mail.ru](mailto:altyn_79@mail.ru), <https://orcid.org/0000-0002-4215-4062>;

Amandykov Madamin Aldamuradovich, Candidate of Technical Sciences, assistant professor, Kazakhstan Engineering and Pedagogical University of Peoples' Friendship, Shymkent, Kazakhstan, e-mail: [Madamin01@mail.ru](mailto:Madamin01@mail.ru), <https://orcid.org/0000-0001-6378-0540>;

Shtern Pavel Gennadevich, Doctor of Technical Sciences, Professor, Yaroslavl State Pedagogical University named after K.D.Ushinsky, Yaroslavl, Russia <https://orcid.org/0000-0002-5513-3068>;

Lukyanova Antonina Vladimirovna, Candidate of Physical and Mathematical Sciences, Yaroslavl State Pedagogical University named after K.D.Ushinsky, Yaroslavl, Russia, <https://orcid.org/0000-0002-7647-4910>;

Koleskin Vladimir Nikolaevich, Candidate of Technical Sciences, assistant professor, Yaroslavl State Pedagogical University named after K.D.Ushinsky, Yaroslavl, Russia, <https://orcid.org/0000-0003-2426-2817>;

Zhumadullayev Daulet Koshkarovich, PhD, senior teacher of the Department of Technological Machines and Equipment, M.Auezov South Kazakhstan State University, e-mail: [daulet\\_ospl@mail.ru](mailto:daulet_ospl@mail.ru), <https://orcid.org/0000-0002-6552-2817>

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