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ИЗВЕСТИЯ

НАЦИОНАЛЬНОЙ АКАДЕМИИ НАУК
РЕСПУБЛИКИ КАЗАХСТАН
АО «Институт топлива, катализа и
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Қазақстан Республикасы Ұлттық ғылым академиясы "ҚР ҰҒА Хабарлары. Химия және технология сериясы" ғылыми журналының Web of Science-тің жаңаланған нұсқасы Emerging Sources Citation Index-те индекстелуге қабылданғанын хабарлайды. Бұл индекстелу барысында Clarivate Analytics компаниясы журналды одан әрі the Science Citation Index Expanded, the Social Sciences Citation Index және the Arts & Humanities Citation Index-ке қабылдау мәселесін қарастыруда. Webof Science зерттеушілер, авторлар, баспашылар мен мекемелерге контент тереңдігі мен сапасын ұсынады. ҚР ҰҒА Хабарлары. Химия және технология сериясы Emerging Sources Citation Index-ке енуі біздің қоғамдастық үшін ең өзекті және беделді химиялық ғылымдар бойынша контентке адалдығымызды білдіреді.

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THE SOLVING OF THE PROBLEM IN THE WORKING ZONE. THE NUMERICAL CALCULATION OF THE MODEL OF THE NIZHNEKAMSK REACTOR FOR THE STYRENE PRODUCTION (PART-3)

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.

Key words: 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 [10- 11] 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 [12-20].

In the *III* domain the equation (16) will be solved by numerical methods [21]. To construct a difference scheme we use a relaxation method [20]. We put the elliptical equation (9) [22] into correspondence with the thermal conductivity equation:

$$\frac{\partial \Psi}{\partial t} = A\frac{\partial^2 \Psi}{\partial r^2} + B\frac{\partial^2 \Psi}{\partial z^2} + 2C\frac{\partial^2 \Psi}{\partial r \cdot \partial z} + 2D, \quad (1)$$

where

$$A = v^2 + v_z^2 = 2(\frac{\partial \Psi}{\partial r})^2 + (\frac{\partial \Psi}{\partial z})^2,$$

$$B = v^2 + v_r^2 = \left(\frac{\partial \Psi}{\partial r}\right)^2 + 2\left(\frac{\partial \Psi}{\partial z}\right)^2,$$

$$C = -v_r \cdot v_z = \frac{\partial \Psi}{\partial r} \cdot \frac{\partial \Psi}{\partial z},$$

$$D = v_z \cdot v^2 = -\frac{\partial \Psi}{\partial r}\left[\left(\frac{\partial \Psi}{\partial r}\right)^2 + \left(\frac{\partial \Psi}{\partial z}\right)^2\right]. \quad (2)$$

The solution of the eq. (9) [22] coincides with stationary ($\partial\Psi/\partial t = 0$) solutions of the eq. (1) at the same boundary conditions.

These conditions are determined by setting values of Ψ function on the *III* boundary which are defined by velocity normal components on the boundary up to a constant. On impenetrable boundaries Ψ = const, an unambiguity and a continuity of Ψ along the boundary is provided by the full mass flow through the boundary equals zero. An arbitrary constant the Ψ function is defined up to does not play any role because equations (1), (2) contain only derivatives of Ψ. To obtain the solution of (1) besides boundary conditions it is necessary to set initial conditions, too. The form of the stationary solution does

not depend on initial conditions but the time for the solution to go to a stationary value (at time-independent boundary conditions) depends heavily on an initial approximation. The eq. (9) differs from the eq. (10) in p.1 [22] only by the last term which does not contain highest derivatives. Hence neither the equation type (elliptical) nor the solution method including a stability criterion of the difference scheme (see formula $\Delta t < \left[\left[\frac{A}{\Delta x^2}\right] + \frac{B}{\Delta y^2}\right]^{-1}$ in [6]) do not differ the case of a plane reactor that is thoroughly considered in p.1 [22].

The solving of a direct problem, i.e. the determination of a velocity field and an evaluation of a pressure field in each reactor zone at specified velocity normal components on Γ_2 and Γ_3 boundaries, does not provide a fulfillment of boundary conditions for the pressure. To find the unique solution that is in accord with all boundary conditions it is necessary to solve an inverse problem such as to find normal components of the velocity on Γ_2 and Γ_3 boundaries that make a minimum of the functional (8) [22].

An introduction of dimensionless variables is made with the help of eqs. (16) and (6) [22]. The reactor length L was selected as a characteristic size. Thus a dimensionless factor of a granular layer resistance R_s in Ergun's law (6)[22] was equal to:

$$R_s = f\frac{v_6^2}{\Delta p} \tag{3}$$

or using the f value (6) in [22] and (3):

$$R_s = 3,5 \cdot \frac{1-\varepsilon}{\varepsilon^3} \cdot L. \tag{4}$$

A numerical calculation was carried out for a model of an industrial reactor for a dehydrogenation of ethylbenzene on K-24 catalyst. The difference of the model from the real reactor was that the distribution manifold of the reactor contains a body of rotation. The element of the side surface of the body was profiled so that the normal component of the velocity is constant at entering the working zone. The model does not have the body of rotation, but the other parameters that are input data for the evaluation are adequate to the industrial unit. Geometrical sizes are: L_0 = 7 m, R_1 = 0,6 m, R_2 = 1,55 m, R_{an} = 1,85 m.

The pipe of the input manifold has a 30% perforation (φ = 0,3) and the pipe of the output manifold has a 3% one (φ = 0,03). The factor of the catalyst layer resistance was defined experimentally, the obtained value f = 8330 kg/m^4. Results of an aerodynamic evaluation are shown in figures 1-2.

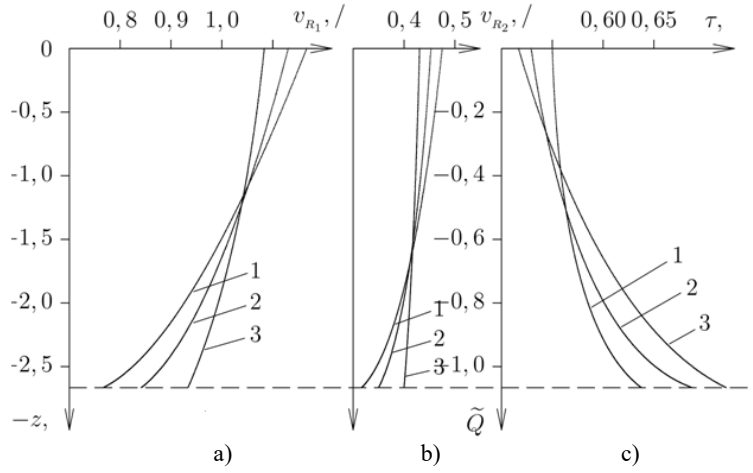

Figure 1 – The influence of the layer resistance on the distribution of the velocity normal components and the stay time on a height: a) the boundary of *I–III* domains; b) the boundary of *III–II* domains; c) the stay time

№	f, kg/m^4	Δp, Pa	Δv_{r_1}, %	Δv_{r_2}, %	ΔT, %
1	3609 (balls d=5 mm)	617	39,9	33,2	33,2
2	4512 (balls d=4 mm)	771	29,1	26,1	25,9
3	9026 (balls d = 2 mm)	1543	14,3	12,1	12,4

Q = 15000 m^3/h, Δp = 1 atm, $\xi_1 = \xi_2 = 0$.

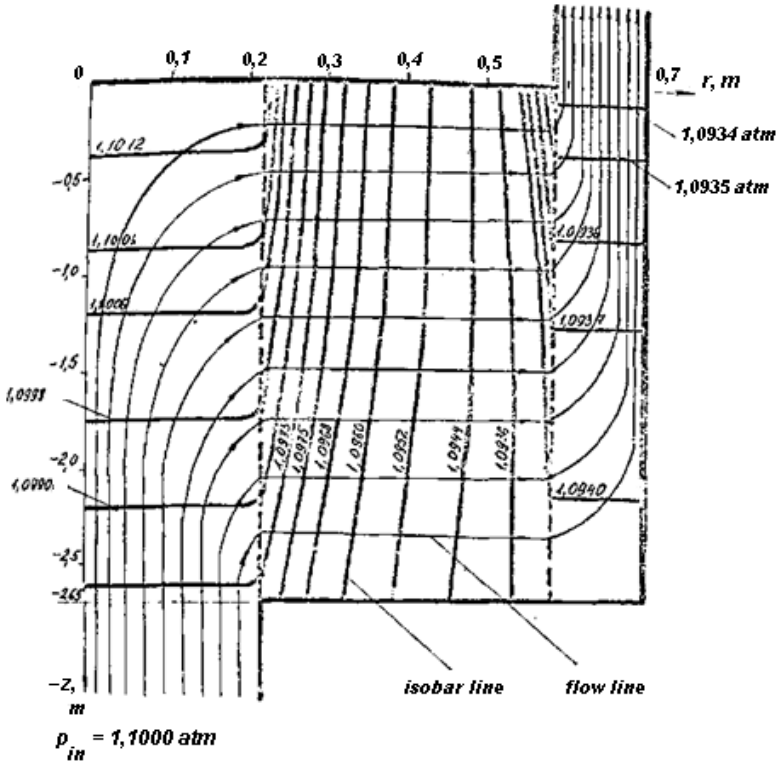

Figure 2 – The evaluated pressure field and flow lines in the model of a radial reactor
f = 4515 kg/m^4; Q = 15000 m^3/h; Δp_l = 0,0076 atm; Δp_{an} = 0,0080 atm.

As the figures show the profile heterogeneity at entering the layer is about 15%. The catalyst layer and the 3% perforation of a shell ring at exiting slightly smooth this heterogeneity (not more than 3%). It follows that at the constant along the reactor height catalyst layer resistance and at accepted geometrical and hydraulic parameters of the reactor the applying of the rotation body and a low perforation degree of the collecting manifold are scarcely advisable to use from the point of view of providing a homogeneous flow in the working zone. This only leads to an increase in a metal consumption of the construction and a pressure drop acting on the reactor, that is an unreasonable increase of economic and energy costs.

The operating experience of industrial units shows that with the time the resistance factor becomes a function of a layer height and increases significantly in its lower part. It proceeds by a vibration of the reactor during an operation first and by an accumulation of a catalyst and technological dust second [1]. It is interesting to make a reactor evaluation with the variable in height hydraulic resistance of the catalyst layer. Thus to describe the flow in *III* domain instead of the eq. (9) [22] it is necessary to use the following equation:

$$(v^2 + v_z^2) \cdot \frac{\partial^2 \Psi}{\partial r^2} + (v^2 + v_r^2) \cdot \frac{\partial^2 \Psi}{\partial z^2} - 2v_r v_z \cdot \frac{\partial^2 \Psi}{\partial r \partial z} + 2v^2 v_z \left(v_r \cdot \frac{\partial lnf}{\partial z} - v_z \frac{\partial lnf}{\partial r} \right) = 0 \qquad (5)$$

Assume that the resistance factor depends only on z and does not depend on r. Then the second term $\left[v_z \left(\frac{\partial \ln f}{\partial r} \right) \right]$ in circle brackets of the fourth term in the eq. (5) [22] turns into zero. An explicit form of $f = F(z)$ dependence is not known (in general case f may depend only upon the time t), therefore at numerical calculations we take a linear dependence of f upon z. A numerical value of f at $z = -L$ was two times greater than at $z = 0$.

The other model parameters were the same. A gas input in the distribution manifold was at $z = -L$ as in a previous variant. In the case the flow heterogeneity is maximal. After adding corresponding changes in the algorithm for solving the problem the numerical calculation was carried out (figures 3 and 4).

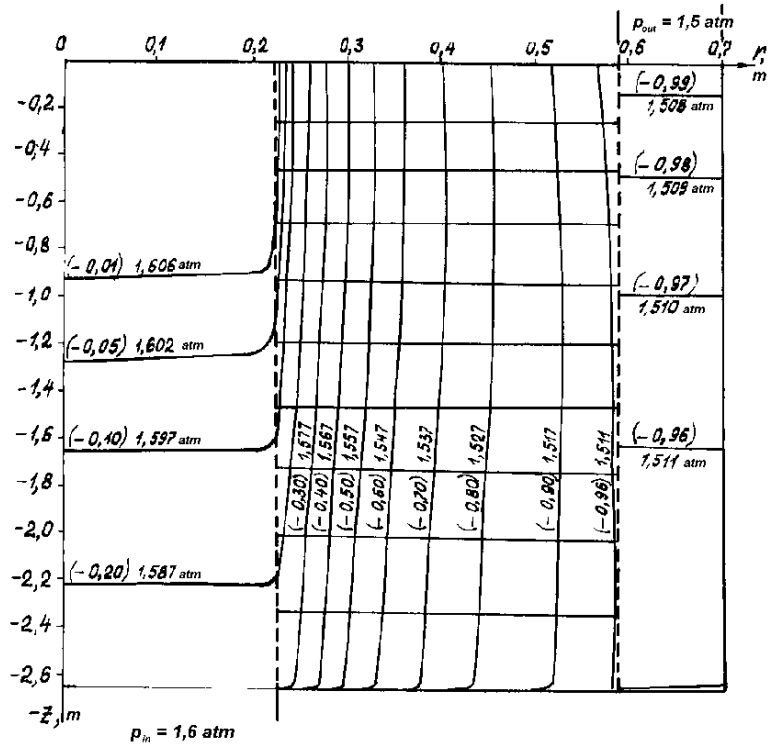

Figure 3 – The evaluated flow lines in *III* domain and the pressure field in the model of Nizhnekamsk reactor with the linear along the height layer resistance: $R_S|_{z=0}$ = 6500, $R_S|_{z=L}$ =13000, L = 7 m, R_1 = 0,6 m, R_2 = 1,55 m, R_{an} = 1,85 m

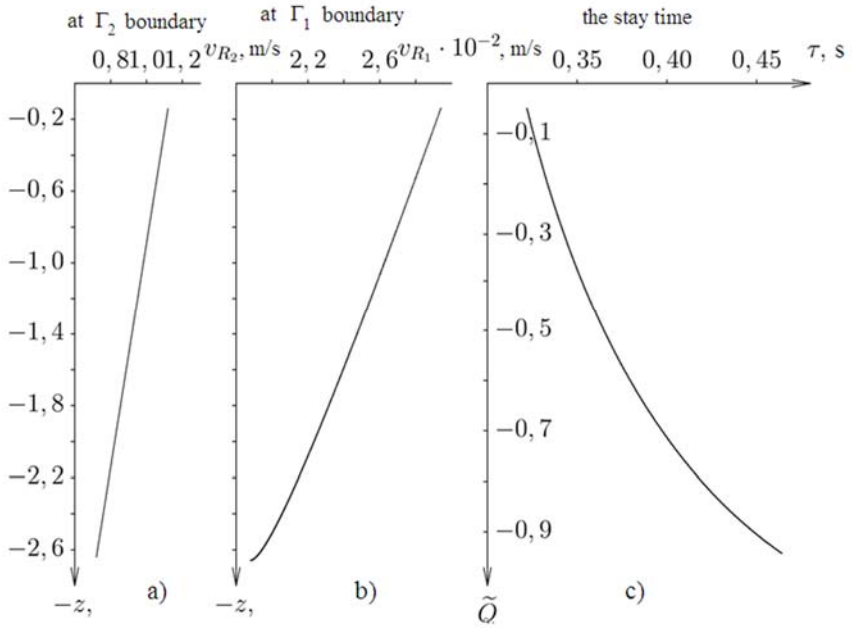

Figure 4 – The distribution of the velocity normal components and the stay time on the unit height at the linearly changing layer resistance: $\boldsymbol{R_S|_{z=0}}$ = 6500, $\boldsymbol{R_S|_{z=L}}$ =13000, L = 7 m, R_1 = 0,6 m, R_2 = 1,55 m, R_{an} = 1,85 m

Results. The evaluation results show that in the upper part of the unit (at z → 0) the radial component of the velocity at entering the working zone and in the catalyst layer increases about 1,4 times and the heterogeneity degree of the velocity profile in the layer is about 50%. This result should be taken into consideration at designing chemical reactors.

So, the hydraulic model and its realization algorithm for radial units with the still granular layer allow make the evaluation of pressures and velocities in the case of an isothermal flow of the incompressible liquid at the square law for a motion resistance.

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ЖҰМЫС АЙМАҒЫНДАҒЫ МӘСЕЛЕНІ ШЕШУ. СТИРОЛ АЛУ ҮШІН НИЖНЕКАМСК РЕАКТОРЫНЫҢ МОДЕЛІН САНДЫҚ ЕСЕПТЕУ (3-БӨЛІМ)

Аннотация. Химиялық технологияның маңызды элементтерінің бірі – катализатордың қозғалмайтын қабаты бар аксиальді немесе радиалды түрдегі реакторларда іске асырылатын гетерогенді каталитикалық үдерістер. Ғалымдар мен өндірушілер назарына осындай байланыс құрылғыларын зерттеу мен қолдануға бірқатар артықшылықтар себеп болған: фазалар бөлімінің жоғары дамыған беті, ағынның жоғары жылдамдығын қамтамасыз ету мүмкіндігі, яғни габариттер мен материал сыйымдылығын азайту, конструкцияның қарапайымдылығы мен пайдаланудағы сенімділік. Байланыс аппараттарының жұмысын жақсартуға қолданыстағы технологияларды жетілдіру және жаңа технологияларды, катализаторлар мен дисперсиялық жүйе құрылымдарын құру есебінен қол жеткізілуі мүмкін. Алайда бірқатар жағдайларда аппараттың жұмыс аймағында ірі масштабты гидродинамикалық біртекті болмауы химиялық, жылу-масса алмасу және басқа да үдерістер тиімділігін арттыру бойынша әрекетті жоққа 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 үдерістің техникалық-экономикалық көрсеткіштері, әдетте, осы үдерісті жобалау сатысында алынған есептік мәннен төмен екендігін растайды. Қазіргі уақытта реактор өнімділігіне әсер ететін себептердің бірі түйіршікті катализатор қабатындағы реагенттер ағынының біртекті еместігі дәлелденген деп санауға болады. Жұмыс қозғалмайтын түйіршікті қабаты бар жазық және радиалды контактілі аппараттарда қысылмайтын сұйықтық ағынын математикалық модельдеуге және осы модельді сандық іске асыру әдістерін құруға арналған. Үш бөліктен тұратын нақты реактор 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 үредістері мен сипаттайтын теңдеулері егжей-тегжейлі қарастырылды.

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

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РЕШЕНИЕ ЗАДАЧИ В РАБОЧЕЙ ЗОНЕ. ЧИСЛЕННЫЙ РАСЧЕТ МОДЕЛИ НИЖНЕКАМСКОГО РЕАКТОРА ДЛЯ ПОЛУЧЕНИЯ СТИРОЛА (ЧАСТЬ 3)

Аннотация. Одними из важнейших элементов химической технологии являются гетерогенные каталитические процессы, реализуемые в реакторах аксиального или радиального типа с неподвижным слоем катализатора. Внимание учёных и производственников к исследованию и применению таких контактных

устройств обусловлено рядом преимуществ: высокоразвитой поверхностью раздела фаз, возможностью обеспечения высоких скоростей потоков и, следовательно, уменьшения габаритов и материалоёмкости, 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.

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