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THE MODELING OF A FLOW IN FLAT AND RADIAL CONTACT UNITS WITH A STILL GRANULAR LAYER. EVALUATIONS OF A CYLINDRICAL REACTOR WITH A RADIAL GAS INPUT AND A FREE OUTPUT (PART 1)

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 [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 [12-13].

The reactor model and the problem setting

Let us produce a scheme of a real reactor as a model that consists of three parts (figure 1). The distribution manifold *I* is a cylindrical pipe of R_1 radius with a blind end and a perforated side surface. The collecting manifold *II* is made by a cylindrical perforated shell of R_2 radius and an outer wall of the unit. The working zone *III* is the still layer of the granular catalyst placed between two perforated coaxial cylindrical surfaces. At PJSC "Nizhnekamskneftekhim" Z-shaped reactors are used for obtaining a styrene, so an input and an output of a gas stream in the model is realized according to Z-shaped scheme.

The pressure drop in radial reactors is not large and it is about some tenth parts of an atmosphere, as a rule. The velocity of the steam-raw mixture is about 1 m/s and Mach number $M \ll 1$, therefore the gas passing the reactor is considered as incompressible.

$$\mathrm{div}\,\boldsymbol{v} = 0 \qquad (1)$$

A stream energy change in *I* and *II* domains on account the gas outflow and inflow through perforated surfaces considerably exceeds energy dissipation due to a viscous friction [14]. Hence the flow in *I* and *II* domains is supposed to be potential:

$$\mathrm{rot}\,\boldsymbol{v} = 0 \qquad (2)$$

Since gas velocities are about 1 m/s we assume a correctness of Ergun's square law and write it down in an invariant form:

$$grad\boldsymbol{p} = -f|v|v \qquad (3)$$

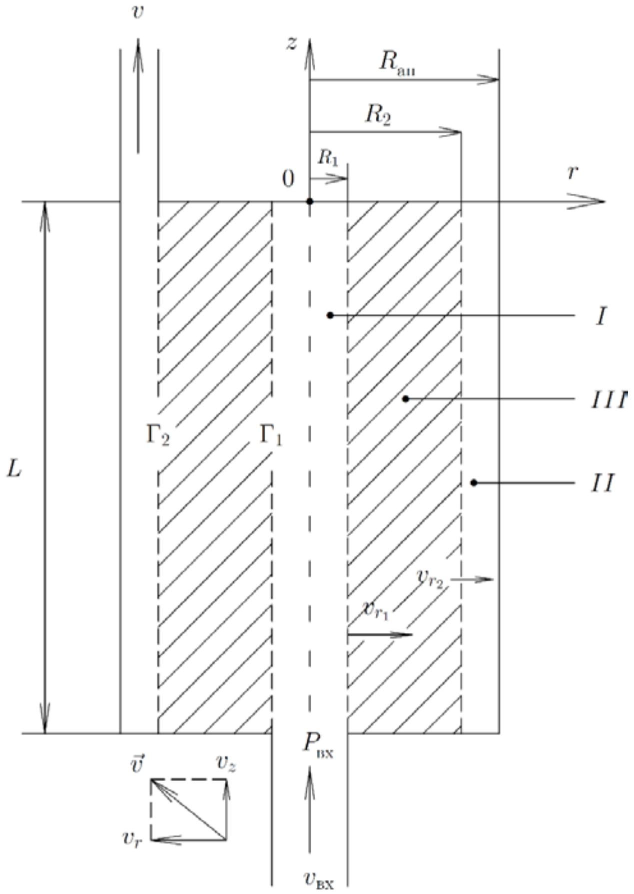

Figure 1 - The unit scheme with the radial gas input

We assume that the flow in units under consideration as axisymmetric, choose the origin and directions of coordinate axis as it is shown in the fig.1 and write down equations (1) – (3) in cylindrical coordinates: the continuity equation

$$\frac{1}{r} \bullet \frac{\partial v_r}{\partial r} + \frac{\partial v_z}{\partial z} = 0 \tag{4}$$

the rotor of the velocity vector

$$\frac{\partial v_r}{\partial z} - \frac{\partial v_z}{\partial r} = 0 \tag{5}$$

Ergun’s law:

$$\frac{\partial p}{\partial r} = -f\ v_r |v|$$
$$\frac{\partial p}{\partial z} = -f\ v_z |v| \tag{6}$$

In *I* and *II* domains the pressure is defined according to Bernoulli's principle:

$$\frac{\rho v^2}{2} + p = const \tag{7}$$

In these equations:
υ_r and υ_z are the radial and axis components of the velocity correspondingly; ρ is a gas density;

$$f = \frac{1{,}75\rho(1-\varepsilon)}{d\varepsilon^3}$$

is a factor of the granular medium resistance; d is an effective diameter of a granule; ε is a medium porosity.

Let Ψ be a flow function, so we write the solution of the equation (1.4) as

$$v_r = \frac{1}{r} \bullet \frac{\partial \Psi}{\partial z}$$

$$v_z = -\frac{1}{r} \bullet \frac{\partial \Psi}{\partial r} \quad (8)$$

by virtue of the pressure mixed derivatives equality and in case of f = const we derive from eq. (6):

$$\frac{\partial^2 \Psi}{\partial z^2}(1+\frac{v_r^2}{v^2}) + \frac{\partial^2 \Psi}{\partial r^2}(1+\frac{v_z^2}{v^2}) - 2\frac{\partial^2 \Psi}{\partial r \partial z} \bullet \frac{v_r v_z}{v^2} + 2v = 0 \quad (9)$$

At Γ_1 and Γ_2 boundaries (see fig. 1) between *I – III* and *III – II* domains correspondingly the continuity conditions for normal components of velocities and pressure are obeyed:

$$v_{r_1} = v_{r_3}, \quad v_{r_2} = v_{r_3},$$

$$p^{(I)} = \Delta p_1 + p^{(III)}, \ p^{(II)} = p^{(III)} - \Delta p_2; \quad (10)$$

where $\Delta p_{1,2}$ is a pressure jump on perforated walls of distributing and collecting manifolds, i.e. on Γ_1 and Γ_2 boundaries, that equals

$$\Delta p_{1,2} = \sigma_{1,2} v_{r_{1,2}}^2 . \quad (11)$$

According to [15-20] the resistance coefficient σ that corresponds to a midrange flow rate through the side surface $\upsilon_{1,2}$ may be expressed by a free section $\varphi_{1,2}$:

$$\sigma_{1,2} = \frac{\rho}{2}[\phi_{1,2}^{-1}(1-\phi_{1,2} + \sqrt{\frac{1-\phi_{1,2}}{2}})]^2, \quad (12)$$

where 1 and 2 indexes are for Γ_1 and Γ_2 boundaries.

If the normal velocity component on Γ_1 and Γ_2 boundaries is set then the full determination of the flow parameters can be conducted for all three domains separately and comes down the solution of elliptical equations like (5) and (9) for the flow function in each domain. The determination of the velocity normal component at Γ_1 and Γ_2 boundaries are made due to the continuity condition for pressure (10) in passing the boundaries. To accomplish this condition at specified velocity normal components a target function is constructed that equals to the mean-square pressure jump at boundaries:

$$\Phi(v_{r_1} v_{r_2}) = \frac{1}{L}\int_{\Gamma_1}(P^{(I)} - P^{(III)} - \Delta P_1)^2 dr + \frac{1}{L}\int_{\Gamma_2} P^{(III)} \text{-} P^{(II)} - \Delta P_2)^2 dz, \quad (13)$$

where L is a length of Γ_1 and Γ_2 (the unit height). The procedure of υ_r and υ_z determination comes down to minimization of the target function Φ.

On eq. (7):

$$P^{(I)} = P_{вх} - \frac{\rho}{2}(v_{r_1}^2 + v_{z_1}^2)$$

$$P^{(II)} = P_{вых} - \frac{\rho}{2}(v_{r_2}^2 + v_{z_2}^2) \quad (1.14)$$

where p_{in} and p_{out} are the full pressure at entering *I* domain and at leaving *II* domain, correspondingly, at $\upsilon_{1,2} = 0$. Since the pressure is recovered up to a constant p_0, the constant should be entered in the number of the target function parameters and p_0 should be determined from the minimum condition, assuming that

$$p^{(III)} = p_0 + \tilde{p}. \quad (15)$$

We select the units of the pressure and velocity measurements so that

$$p_{\text{вх}} - p_{\text{вых}} = 1$$

$$v_B = \sqrt{\frac{2(p_{BX} - p_{BЫX}}{\rho}} = 1 \quad (16)$$

and set the value

$$q_1 = p_{in} - p_0 \quad (17)$$

and rewrite eq. (13) in account for (11), (14) and (15 – 17) as

$$\Phi\left(\nu_{r_1}, \nu_{r_2}\right) = \frac{1}{L}\int_{\Gamma_1} \left[\tilde{p} + \left(1 + \tilde{\sigma}_1\right)\nu_{r_1}^2 + \nu_{z_1}^2 - q_1\right]^2 dx + \frac{1}{L}\int_{\Gamma_2} \left[\tilde{p} + \left(1 - \tilde{\sigma}_2\right)\nu_{r_2}^2 + \nu_{z_2}^2 - q_1 + 1\right]^2 dz \quad (18)$$

where $\tilde{\sigma}_{1,2} = \frac{2\sigma_{1,2}}{\rho}$ is a dimensionless coefficient of a perforation resistance, that in general case may be a function of *z*.

Results. So, the problem solution method is a searching for υ_{r_1} and υ_{r_2} that make a minimum of the functional (18). The solution of the direct task in *I* domain (the distribution manifold) is shown in [17] and looks like:

$$\pm\frac{1}{\pi}\int_{z-h}^{z+h} \frac{(z-\bar{z})}{\Delta^2 + (z-\bar{z})^2} \bullet v_{1,2}(\hat{z})d\ddot{z} = \frac{1}{\pi} \bullet \frac{\partial v_1}{\partial \bar{z}}\Big|_{\bar{z}=z} \bullet \int_{z-h}^{z+h} \frac{(z-\bar{z})^2}{\Delta^2 + (z-\bar{z})^2} d\bar{z} = \pm\frac{2h}{\pi} \bullet \frac{\partial v_{1,2}}{\partial \bar{z}}\Big|_{\bar{z}=z} \quad (19)$$

This equation allows to reach an accuracy $O(h^2)$ in the determination of the velocity tangential component and pressure on boundaries of *I, III* and *III, II* domains.

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АҒЫНДЫ ҚОЗҒАЛМАЙТЫН ТҮЙІРШІКТІ ҚАБАТЫ БАР ЖАЗЫҚ ЖӘНЕ РАДИАЛДЫ БАЙЛАНЫС АППАРАТТАРДА МОДЕЛЬДЕУ. ГАЗДЫ РАДИАЛДЫ ЕНГІЗУМЕН ЖӘНЕ ЕРКІН ШЫҒАРУМЕН ЦИЛИНДРЛІК РЕАКТОРДЫ ЕСЕПТЕУ (1-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 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 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 сұйықтық-тың ағынын математикалық моделдеуге 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 олардый 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.

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МОДЕЛИРОВАНИЕ ТЕЧЕНИЯ В ПЛОСКИХ И РАДИАЛЬНЫХ КОНТАКТНЫХ АППАРАТАХ С НЕПОДВИЖНЫМ ЗЕРНИСТЫМ СЛОЕМ. РАСЧЕТ ЦИЛИНДРИЧЕСКОГО РЕАКТОРА С РАДИАЛЬНЫМ ВВОДОМ ГАЗА И СВОБОДНЫМ ВЫХОДОМ (ЧАСТЬ 1)

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 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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