ХИМИЯ

THE NUMERICAL MODELING OF A FLOW IN PLANE AND RADIAL CONTACT UNITS WITH A STILL GRANULAR LAYER

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Abstract. Attempts of strict mathematical modeling heterogeneous media that are made in some investigations are necessarily limited by some prior specified theoretical schemes and this fact requires many experimental data for a practical realization. The analysis of known works shows that a physical essence of processes arising at a liquid or gas motion in contact units is insufficiently studied. In articles dealt with a mechanics of disperse systems, issues of constructing computational and theoretical models of concrete industrial devices that would took into account basic experimental facts and sufficiently simple from engineer's point of view are poorly reflected.

The experience of an operation of chemical reactors shows that technical and economic indicators of an industrial process are as a rule lower than evaluated values that were obtained during a design step. Now it can be considered proven that one of the reasons that affects a reactor capacity is heterogeneity of a reagent flow in a granular catalyst layer.

In some works [1], [2], [3], [4] computational and theoretical models of a filtration mode of a liquid and gas flow in the still granular layer that is in a stress-strain state under a load from the carrier phase were proposed. Results calculated according these models are in a qualitative agreement with experimental data and a large-scale heterogeneity of a velocity profile corresponds to a scale of granular layer structure heterogeneity. But using Darcy's law or Ergun's equation to describe a motion of the carrier phase in an inhomogeneous granular medium requires a justification because a formation of boundary layers is possible along borders of the areas with a different permeability.

In radial units with the still granular layer (SGL) it is considered that the large-scale heterogeneity of a radial component of the velocity in the granular layer is caused mostly by reagent flow features in distributing and collecting manifolds. So a majority of works dealt with such units investigates a flow with a suction or injection in channels with perforated walls. A distribution along a distributing manifold length of a cross-section average value of an axial component of the velocity flow was determined by Meshcherskiy's equation, an energy approach, models of potential flows in [5], [6], [7] an so on. The main task was to provide the stable radial velocity at entering the granular layer.

From the above review a conclusion can be made that physical features of the liquid and gas motion in SGL are poorly explored both theoretically and experimentally. For example, conflicting results of measuring the velocity profile in axial units with SGL, a variety of motion equations used for calculation, a lack of information about a volume structure of the granular layer that arises during loading the unit and so on testify it.

So there is a necessity to construct computational and theoretical models of concrete industrial units that would took into account basic properties of a technological process and were sufficiently simple engineer's solutions for designing new technological systems.

Keywords: chemical reactor, steam-raw mixture, reagent, large-scale heterogeneity, catalyst, perforated channel, manifold, working area, velocity field, pressure field

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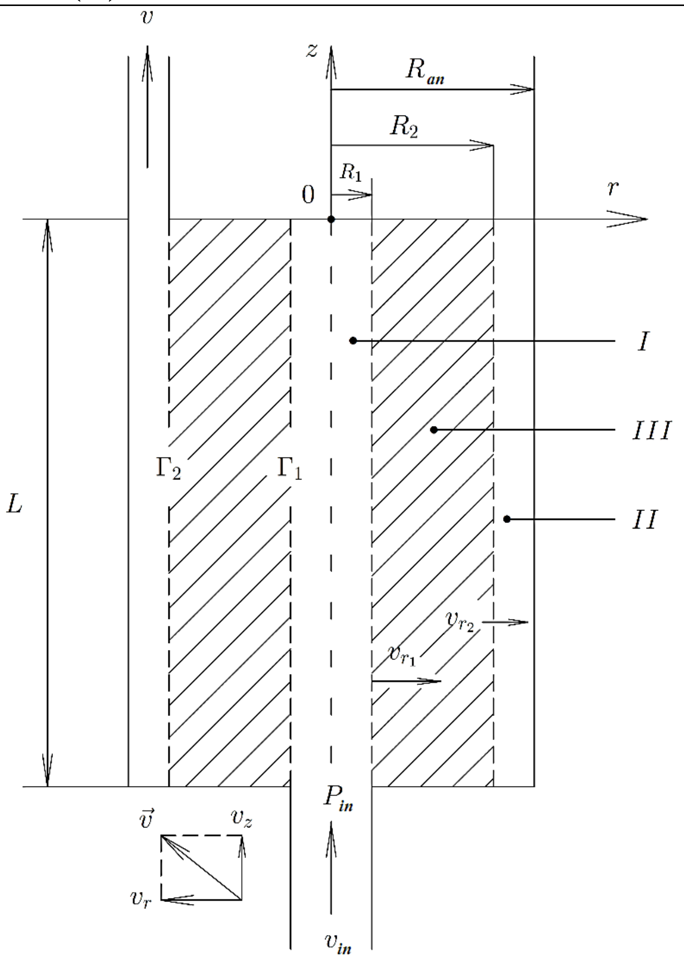

Fig. 1. The scheme of the unit with a radial gas input

In [8] the mathematical modeling of an incompressible liquid flow in plane and radial contact units with the still granular layer was developed and methods of a numerical realization of the model were shown.

The flow area in the unit can be conditionally split into three sub-areas (fig. 1) — distributing *I* and collecting *II* manifolds and working area *III*, that is the still granular layer placed between two coaxial perforated cylindrical shells. A pressure drop in radial reactors is not large and is about tenths of the atmosphere.

The velocity of the steam-raw mixture is about 1 m/s and Mach number *M* << 1, therefore the gas passing the reactor can be considered as incompressible.

It is known, for instance [9], [7], that near the axial zone of the channel an impulse flux for the flow with the powerful suction (the distributing collector) and the injection (the collecting manifold) is several orders of magnitude higher than the viscous flow. The liquid near the axial zone looks like almost the ideal one and for a core of the flow a stream in *I* and *II* areas can be considered as potential one. The motion of the incompressible liquid in the working area *III* is determined by Ergun's law where a resistance term that is linear over the velocity is neglected.

As a result we obtained a system of equations to find a velocity and pressure fields:
for a total flow area:

$$div\ \upsilon = 0 \tag{1}$$

for *I* and *II* areas

$$rot\ \upsilon = 0 \text{ and } \frac{\rho v^2}{2} + p = const \tag{2}$$

for the working area *III*

$$grad\ p = -f \cdot |\upsilon| \cdot \upsilon \tag{3}$$

After writing down the solution of eq. (1) through a current function Ψ as

$$\upsilon_r = \frac{1}{r} \cdot \frac{\partial \Psi}{\partial z} \text{ and } \upsilon_z = -\frac{1}{r} \cdot \frac{\partial \Psi}{\partial r} \tag{4}$$

we can find a second order partial differential equation of the elliptic type for every area: *I*, *II* and *III*. So, for instance, the equation for *III* area looks like:

$$(\upsilon^2 + \upsilon_z^2)\frac{\partial^2 \Psi}{\partial r^2} + (\upsilon^2 + \upsilon_r^2)\frac{\partial^2 \Psi}{\partial z^2} - 2\upsilon_r \upsilon_z \frac{\partial^2 \Psi}{\partial r \partial z} + 2\upsilon^2 \upsilon_z \left(\upsilon_r \frac{\partial\, \ln f}{\partial z} - \upsilon_r \frac{\partial\, \ln f}{\partial r}\right) = 0 \tag{5}$$

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

$$\upsilon_{r_1} = \upsilon_{r_3}\ \upsilon_{r_2} = \upsilon_{r_3}$$

$$p^{(I)} = \Delta p_1 + p^{(III)}\ p^{(II)} = p^{(III)} - \Delta p_2\,, \qquad (6)$$

where $\Delta p_{1,2}$ is the pressure drop at perforated walls of the distributing and collecting manifolds; it is equal $\Delta p_{1,2} = \sigma_{1,2}\upsilon_{r_{1,2}}^2$ and $\sigma_{1,2}$ is the resistance coefficient that corresponds to an average over the manifold side surface velocity $\upsilon_{r_{1,2}}$ which may be in general a function of *z* f the normal component of the velocity at Γ_1 and Γ_2 boundaries is specified then the full determination of the flow parameters can be conducted for all three areas separately and comes down to solving the above differential equations for the current function in every area. That is a *direct problem*. Matching the obtained solutions is made by determining the normal components of the velocity at Γ_1 and Γ_2 boundaries that is accomplished using the continuity condition for the pressure (6) at passing these boundaries. To fulfill this condition at specified normal components of the velocity υ_{r_1} and υ_{r_2} the target function Φ is constructed that equals to the average square of the pressure drop at the boundaries:

$$\Phi(\upsilon_{r_1}, \upsilon_{r_2}) = \frac{1}{L}\int_{\Gamma_1}\left(p^{(I)} - p^{(III)} - \Delta p_1\right)^2 dz + \frac{1}{L}\int_{\Gamma_2}\left(p^{(III)} - p^{(II)} - \Delta p_2\right)^2 dz, \qquad (7)$$

where *L* is the length of Γ_1 and Γ_2 boundaries (the unit height). The procedure of the determination of υ_{r_1} and υ_{r_2} comes down to the target function Φ minimization. It is an *inverse problem*. The solution of the direct problem in *I* and *II* areas was obtained analytically with Green's function means [10] and the solution of the direct and inverse problems in *III* area was carried out with the help of numerical techniques on a computer. Results of the evaluation of the suggested hydrodynamic model carried out for various particular types of radial units are in good agreement with published ones and experimental data obtained in [8].

With the help of alternative calculations of the model and theoretical analysis of some particular types of radial units we have investigated the influence of the layer resistance on the distribution of relative values of the axial component of the velocity in the distributing manifold, radial components of the velocity at Γ_1 and Γ_2 boundaries (see fig. 1) and the stay time along the unit height.

We determined the dependence of a coefficient for decreasing consumption:

$$\eta = \frac{\upsilon_{in} - \upsilon_{in}^p}{\upsilon_{in}} \qquad (8)$$

and a degree of the nonuniformity of the radial velocity profile at Γ_1 boundary

$$\xi = \frac{\upsilon}{\frac{\upsilon_{in}}{r_{1\ max}{}^{min}_{r_2}}} \qquad (9)$$

of a dimensionless pressure drop $\Delta\tilde{p}_k = \frac{\Delta p_k}{\Delta p_{an}}$ in the distributing manifold. In the range of $\Delta\tilde{p}_k = 0 \div 2{,}5$ these dependences can be presented by linear equations

$$\eta = \frac{1}{6}\Delta\tilde{p}_k;\ \xi = \frac{1}{2}\Delta\tilde{p}_k. \qquad (10)$$

The obtained equations have a high degree of a generality because they set a relationship between dimensionless values and do not depend upon geometrical sizes of units and its consumable characteristics in a wide range of these magnitudes. Besides, the pressure drop in the manifold $\Delta\tilde{p}_k$ for industrial units (for example, chemical reactors) lies as a rule inside the range that was mentioned above. In the assumption that the total pressure drop that occurs at inner and outer perforations and at the granular layer (see fig.1) is much higher than the drop along manifolds, i.e. $\frac{\Delta p_k}{\Delta p_{an}} << 1$, and at the condition f = const we have made the theoretical evaluation of the radial unit with a low degree of the inhomogeneity flow. On the base of the obtained solution we have explored a particular case that is a device with an output in the barometric environment and without the outer perforated shell at Г2 boundary. The analytical solution of the problem results in (10) also.

So, equations (10) that are obtained by a strict theoretical way are in good agreement with the results of a numerical experiment that in its turn determined the limits of theoretical model applicability. It should be noted that numerical calculations confirm the validity of equations (10) not only for units with the flow output into the atmosphere but also for any reactor, i. e. any unit containing the collecting manifold with a perforated shell.

All results that were derived in IV chapter of [8, p. 270] allow developing construction principles for an engineer method of the radial unit with the still granular layer design. The method permits to carry out an estimate of optimal options of a constructive implementation for devices of various technological purposes and to define its consumption characteristics upon the specified total pressure drop, the inhomogeneity flow degree and some technological and hydraulic parameters. The detailed definition of velocity and pressure fields in all areas of the selected type of the unit is accomplished by means of a numerical calculation on the computer according to the proposed mathematical model.

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