MERIDIONAL CIRCULATION OF LIQUID DURING MIXING IN REACTORS WITH STIRRERS AND DEFLECTING BAFFLES

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A mathematical model has been proposed for the calculation of the circulating flow of liquid in reactors with baffles and stirrers, based on the energy balance in the reactor. A semiempirical relationship has been obtained between the circulation rate and the design characteristics of the reactor and the stirrer for a developed turbulent regime. The results of the calculations have been compared with the experimental data.

The meridional circulation of a liquid is one of the main factors, characterizing the hydrodynamic conditions, and which determine the mixing processes in reactors with stirrers, equipped with deflecting baffles. The circulation rate is used as the basic parameter when describing different mixing problems within the framework of determined as well as stochastic models of transport on the macroscale [1], heat exchange [2], micromixing [3], etc.

The circulation rate Q as function of the mixing conditions is usually expressed in the form [4]

$$Q=k_Q n d_м^3=2k_q n d_м^3. \tag{1}$$

The values of the rate coefficient $k_Q$ for turbine stirrers, quoted by different authors, vary within the limits 1.0-2.5. In the first studies, devoted to the experimental measurement of circulation and generalized in [4], it was assumed that $k_Q$ depended only on the type of stirrer; the influence of the relative dimensions of the stirrer and the reactor on the coefficient was neglected.

An experimental correlation has been proposed in [5] between the circulation rate and the design characteristics of turbine and radial-blade stirrers:

$$Q=0{,}9nd_м^3(d_м/D)^{-1{,}5}(h_b/D)^{0{,}5}z_b^{0{,}31}=2q. \tag{2}$$

Equation (2) was obtained for a limited range of characteristics of the reactor: The height of filling of the reactor was equal to its diameter, the properties of the medium were maintained unchanged, and the stirrer was positioned at half the filling height.

The present study is devoted to the development of a more general method for the calculation of the circulation rate of the stirred medium, which takes into account changes in the design and dimensions of the reactor with stirrer within limits which are characteristic for industrial-scale equipment [6].

Such a method can be based on the analysis of the energy balance in the reactor. Having in mind an approximated solution of the problem, let us consider the circulation contour as being symmetrical with respect to the axis of the reactor and consisting of two linear sections of ascending and descending flow and of two zones of flow reversal (Fig. 1).

At an established regime the energy $E_c$, lost by the liquid in a unit of time when traveling in the circulation contour, can be presented as the sum of two components: the energy spent to overcome the friction forces in the linear sections $E_1$ and to overcome local resistances $E_2$:

$$E_c=E_1+E_2. \tag{3}$$

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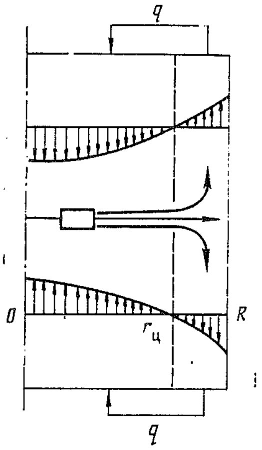


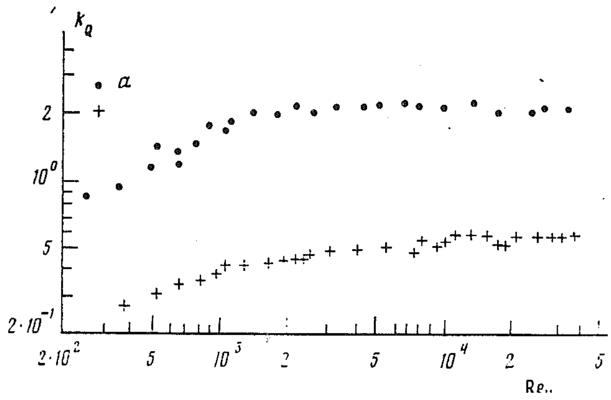


Fig. 1 Fig. 2

Fig. 1. Scheme of the flow structure in reactors with deflecting baffles.

Fig. 2. Coefficient of circulation rate as function of $Re_c$: a) open turbine stirrer ($\xi_m = 8.4$); b) twin-blade stirrer ($\xi_m = 0.88$).

Since energy losses for friction at the walls are negligible at the conditions under consideration, $E_1$ can be taken as equal to the dissipation of energy of turbulent movement, due to the presence of a gradient of axial velocity:

$$E_1 = \int\limits_{V_c} \rho\varepsilon\, dV.$$

By using the "law of two thirds" of Kolmogorov and Obukhov

$$\varepsilon \sim (v')^3/l$$

and by expressing the pulsation rate v' and the length of the mixing path $\ell$ according to Prandtl by

$$v' = l\left|\frac{dW}{dr}\right|_{av}, \qquad l = \varkappa R,$$

we obtain the first approximation

$$E_1 = \int\limits_{V_c} \rho\varkappa^2 R^2 \left|\frac{dW}{dr}\right|_{av}^3 dV,$$

$$\left|\frac{dW}{dr}\right|_{av} = \frac{2}{R^2}\int\limits_0^R \left|\frac{dW}{dr}\right| r\, dr.$$

$E_2$, the capacity dissipated in four turns of the axial flow by 180°, can be expressed through the average velocity of axial flow $W_{av}$ and the coefficient of local resistance $\xi_t$:

$$E_2 = \xi_t \rho\pi R^2 W_{av}^3,$$

in accordance with (3) this gives

$$E_c = \frac{8\pi\varkappa^2 H\rho}{R^2}\left[\int\limits_0^R \left|\frac{dW}{dr}\right| r\, dr\right]^3 + \pi\rho\xi_t R^2 W_{av}^3. \tag{4}$$

In order to determine the average radial gradient of axial velocity we can use the equation for the velocity profile*

$$W(r)=\frac{4q}{\pi R^2}\left(\frac{2r^2}{R^2}-1\right), \tag{5}$$

which was obtained in [7], starting from the flow scheme given in Fig. 1. From this equation it follows that

$$W_{av}=2q/(\pi R^2); \tag{6}$$

$$\frac{dW}{dr}=\frac{16q}{\pi R^4}r. \tag{7}$$

Substitution of (6) and (7) in (4) gives

$$E_C=\frac{q^3}{\pi^2 R^4}\rho\left(\frac{2^{15}}{27}\varkappa^2\frac{H}{R}+8\xi_t\right). \tag{8}$$

The value of $E_C$ represents only a fraction $\varphi$ of the total capacity N, spent for the mixing:

$$E_C=\varphi N=\varphi k_N n^3 d_м^5 \rho. \tag{9}$$

Assessments calculated from (8) by using the values $\xi_t = 2$ [8], $\varkappa = 0.1$,† and experimental data for the circulation rate [5]; the values of $\varphi$ lie within the limits 0.05 to 0.25 which are of the same order of magnitude as the experimental assessments [10, 11].

By solving (8) and (9) with respect to q and by using the equation of the circulation rate in the traditional form (1) we obtain:

$$k_q=0{,}03\left[\frac{\pi^2 k_N \varphi (D/d_м)^4}{(H/D)\varkappa^2+0{,}0033\xi_t}\right]^{0{,}33}. \tag{10}$$

In order to obtain $\varphi$ let us assess the capacity, spent in the interaction of the liquid with the blades. According to [7] the force applied to the elementary section of the blade length in the flow is given by:

$$dF=\xi_t \rho h_b (u^2/2)\,dr,$$

where $u = (\omega_0 r - v)$ is the relative velocity of the flow around the blade.

Having determined the energy spent in a unit of time in the case of flow around the elementary section of the blade in the form

$$dE_м=\xi_b \rho \frac{h_b}{2} z_b u^3\,dr$$

for a stirrer with the number of blades $z_b$, we obtain

$$E_м=\xi_b \rho \frac{h_b}{2}\int_{r_{int}}^{r_0} u^3\,dr. \tag{11}$$

For a reactor with deflecting baffles the peripheral speed of the liquid v can be taken with sufficient approximation [7] to be constant and equal to

$$v_{av}=\pi n d_м \frac{0.33-\sqrt{0.11-0.25(0.5-k_{int})}}{0.5-k_{int}}, \tag{12}$$

*Regardless of the simplifications made when developing it, Eq. (5) describes satisfactorily the experimental data.

†The value $\varkappa = 0.1$ corresponds to the results of the study of turbulent flow in tubes [9] and in reactors with stirrers without internal devices [7].

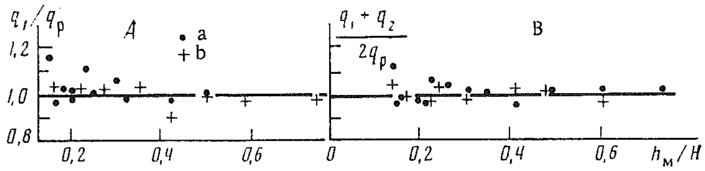


Fig. 3. Circulation rate in the upper contour (A) and summary rate (B) as function of the height of installation of the stirrer: a) open turbine stirrer; b) twin-blade stirrer.

where

$$k_{int} = \frac{(R/r_0)^3}{\xi_м} \sum_{z_{int}} \xi_i f_i \frac{r_i}{R^3};$$

$z_{int}$ is the number of internal devices; $r_i$ is the radius of installation of the i-th internal device, m; $f_i$ is the surface area of the projection of the i-th internal device on the meridional plane, m$^2$; $\xi_i$ is the coefficient of resistance of the i-th internal device.

By introducing the denotations

$$\bar{r}_{int} = r_{int}/r_0; \quad \bar{v}_{av} = v_{av}/(\pi n d_м)$$

and by taking into account that for blade and open turbine stirrers $\bar{r}_{int} \leq 0.5$, we obtain after integration of (11) the expressions for $E_m$ and $(1 - \varphi)$:

$$E_м = \frac{\rho \xi_м \pi^3}{8} n^3 d_м^5 [0.25 - \bar{v}_{av} + 1.5\bar{v}_{av}^2 - \bar{v}_{av}^3 (1 - \bar{r}_{int})];$$

$$1 - \varphi = \frac{E_м}{N} = \frac{\pi^3 \xi_м}{8k_N} [0.25 - \bar{v}_{av} + 1.5\bar{v}_{av}^2 - \bar{v}_{av}^3 (1 - \bar{r}_{int})],$$

where $\xi_m = \xi_b z_b h_b / r_0$ is the coefficient of resistance of the stirrer.

By taking into account that $k_N$ is related to $v_{av}$ by the correlation [7]

$$k_N = 3.87 \xi_м (0.25 - 0.67\bar{v}_{av} + 0.5\bar{v}_{av}^2),$$

we obtain

$$\varphi = \frac{\bar{v}_{av}^3 (1 - \bar{r}_{int}) - \bar{v}_{av}^2 + 0.33\bar{v}_{av}}{0.25 - 0.67\bar{v}_{av} + 0.5\bar{v}_{av}^2}. \qquad (13)$$

Equations (10), (13) in combination with (12) for the calculation of $v_{av}$ form a closed system and allow one to calculate the circulation rate of the liquid in reactors with stirrers of different size and ratios, based on data on the resistance coefficients of the blades, given in [7, 12].

The obtained correlations were verified experimentally by using the method given in [13], which involves measurement of the average circulation time of a tracer particle with zero buoyancy. During the experiment we measured the number of passages of the tracer particle through the turning zone (from the central branch of the contour to the peripheral branch, Fig. 1) in the time $\tau$; the liquid flow rate was calculated from the equation

$$Q = V_c / \tau_{av}, \qquad (14)$$

where $\tau_{av} = \tau/m$; m is the number of passages in the time $\tau$.

It must be pointed out that the use of Eq. (14) is justified when the probability that the particle will fall into a given point is equal. That this condition was satisfied in all measurements made, was checked by establishing that the distribution of the frequency of passages corresponded to Poisson's distribution [15]. The checking was based on Pearson's number.

Twin-blade and open turbine stirrers were used in the tests [14]. The geometrical parameters of the reactors and stirrers were varied within the following limits:

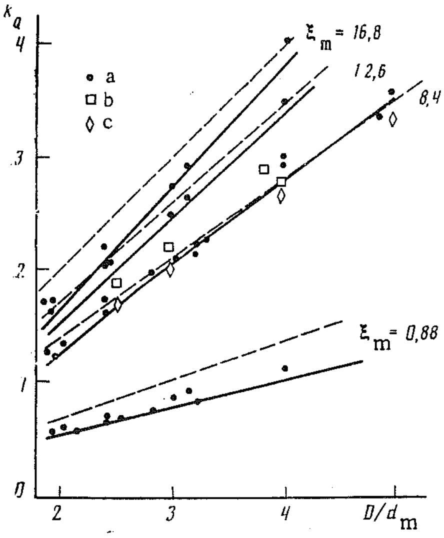


Fig. 4

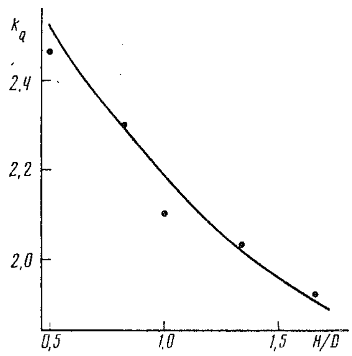


Fig. 5

Fig. 4. $k_Q$ as function of $D/d_m$: broken lines: calculated from (1), (2), solid lines: from (10); a) experimental data; b) data from [16]; c) data from [17], recalculated according to [19].

Fig. 5. $k_Q$ as function of H/D for an open turbine ($D/d_m$ = 3, $\xi_m$ = 8.4): the points are experimental data, the solid curve has been calculated from (10).

$$H/D=0.5\ldots1.67;\ n_b=4;\ B/D=0.1;\ D/d_м=1.8\ldots6;$$
$$h_b/d_м=0.1\ldots0.4;\ D=160;\ 240;\ 300;\ 500\ мм;\ h_м/H=0.1\ldots0.75.$$

where $n_b$ is the number of baffles; B is the width of the baffle, m; $h_m$ is the height of installation of the mixer above the bottom, m.

The working media used were water, glycerol, and aqueous glycerol solutions (viscosity $\mu$ = 1-600 cP); polystyrene spheres with a diameter of 3.5-5 mm and a density $\rho$ = 1000 kg/m$^3$ served as the tracers. The time interval $\tau$ was selected in every concrete case so, that the total number of passages m was not less than 500.

The results of the measurements allowed us to establish the boundaries of the developed turbulent regime of mixing which corresponded to the absence of an influence of the viscosity of the medium on the circulation rate. The data in Fig. 2 show that a noticeable influence of the viscosity of the medium is observed only at relatively high $Re_c$ values ($Re_c$ = 8000 for a twin-blade stirrer and 3000 for a turbine stirrer), corresponding to Re = 1300.

In this region of flow regimes a change in the position of the centers of circulation in the reactor was observed in the tests described in [5], in our tests a deviation of the distribution of the circulation frequency of the tracer particle from Poisson's law.* It must be pointed out that in the case of reactors equipped with stirrers without deflecting baffles the values of the Reynolds number, corresponding to the onset of the turbulent regime, were close to 1500 [7].

In Fig. 3 the measured rate in the upper contour $q_1$ and the summary rate ($q_1 + q_2$) has been compared with the calculated values $q_c$, obtained from Eq. (10). It follows from these data that the circulation rate in the zones above and below the level of installation of the stirrer are equal and practically independent of the height of installation of the stirrer above the bottom.

*In this case, in order to find the circulation rate, $V_c$ in (14) must be replaced by the active volume, determined visually.

In Figs. 4 and 5 the experimental values of the coefficient of circulation rate in a developed turbulent regime ($Re_c > 10^4$) are compared with those calculated from (10). Data are presented of measurements made in [16, 17] and curves calculated from Eq. (2). The graphs show that the proposed method for the calculation of the circulation rate offers a satisfactory agreement with the experimental data. Its precision is not inferior to that of the experimental Eq. (2) but is applicable to a wider range.

At the intermediate stages of the development of (10) the energy spent for the movement of the liquid in the circulation contour was determined from Eq. (5) which represents the approximation of the radial profile of axial velocity by a parabola. Such a description and the hydrodynamic model on which it is based are not unique; the literature contains also other models and approximated analytical expressions [18]. It must be pointed out therefore that the proposed calculation procedure can be used in combination with any other equation which describes with sufficient precision the radial distribution of the axial velocity. For example, the use of the velocity profile [18]

$$W=\frac{W_0}{2}\left(3\frac{r^4}{R^4}-1\right),$$

where $W_0$ is the velocity at $r = R$, gives

$$k_q=0.03\left[\frac{\pi^2 k_N \varphi (D/d_m)^4}{1.6(H/D)\varkappa^2+0.0036\xi_t}\right]^{0,33}. \qquad (15)$$

It can be seen that this expression differs from (10) only in the numerical coefficients which slightly exceed unity. The difference between the values of $k_q$, calculated from Eqs. (10) and (15), does not exceed 17%.

## NOTATION

$d_m$ is the diameter of the stirrer, m; D is the diameter of the reactor, m; $h_b$ is the height of the stirrer blade, m; H is the height of filling of the reactor, m; $k_N$ is the capacity coefficient; $k_q$ is the circulation rate coefficient; $\ell$ is the length of the mixing path; n is the rotation frequency of the stirrer, rpm; N is the power spent for the mixing, W; q is the circulation rate in the contour, located above the plane of rotation of the stirrer, $m^3$/sec; r is the current radius, m; $r_{int}$ is the radius of the inner edge of the stirrer blade, m; $r_0$ is the radius of the stirrer, m; R is the radius of the reactor, m; u is the relative velocity of flow around the blade, m/sec; v, $v_{av}$ is the peripheral and average peripheral speed of the liquid, m/sec; v' is the pulsation velocity, m/sec; $V_c$ is the volume of the reactor, $m^3$; W, $W_{av}$ is the velocity and average velocity of axial flow, m/sec; $z_b$ is the number of blades of the stirrer; $\varepsilon$ is the rate of energy dissipation in a unit mass of liquid, W/kg; $\varkappa$ is a proportionality coefficient; $\mu$ is the dynamic viscosity of the liquid, Pa·sec; $\xi_b$, $\xi_m$ are the coefficients of resistance of the blade and the stirrer; $\xi_t$ is the coefficient of resistance of the turn of the axial flow by 180°; $\rho$ is the density of the liquid, $kg/m^3$; $\omega_0$ is the angular velocity of rotation of the stirrer, rad/sec; $Re_c = \rho n d_m^2/\mu$ is the centrifugal Reynolds number; $Re = \rho W_{av} R/\mu$ is the Reynolds number.

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# OPTIMIZATION OF SHELF-TYPE REACTORS WITH COMBINED HEAT EXCHANGE FOR RANDOM CHEMICAL REACTIONS

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The problem of optimization of reactions having adiabatic catalyst beds and a combined system of heat exchange between them is examined. The requisite optimality factors are derived, making allowance for the limitations of the minimum and maximum temperatures in the bed. It is shown that these data can be used for real reactors under different optimization situations.

Reactors having static catalyst beds are important units for many chemical-technological processes, including large-scale production of ammonia, methanol, hydrogen, sulfuric acid, etc. Optimization of the apparatus will make it possible to raise the efficiency of the units being designed and to intensify the functioning ones.

The optimization problem consists in the following:

1) to find the optimal technological parameters (temperature at the shelf inlet or dimensions of the bypasses) which ensure maximum productivity for the functioning apparatus of a specific design (shelfwise catalyst distribution and heat-exchange system);

2) to find for the apparatus being designed the optimal shelfwise catalyst distribution and the same technological parameters as for the functioning reactor which maximize the unit productivity of the catalyst.

The problem of optimization of some reactor designs [having intervening heat-exchangers [1, 2] with cold gas injection (bypasses)] between the shelves [3-10], with a bypass after the first bed and heat-exchangers after the others [11] was examined in the literature. The problem of synthesis of an optimal design of a reactor consisting of adiabatic shelves and heat-exchangers is solved in [12]. However, from this set of designs it is not always possible to select the optimum one, especially the one that combines heat-exchangers and cold

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