ISSN 1070-4272, Russian Journal of Applied Chemistry, 2009, Vol. 82, No. 4, pp. 741–747. © Pleiades Publishing, Ltd., 2009.
Original Russian Text © A.B. Golovanchikov, A.A. Shagarova, N.A. Dul'kina, 2009, published in Khimicheskaya Promyshlennost', 2009, Vol. 86, No. 1, pp. 37–44.

MODELING AND CALCULATION OF TECHNOLOGICAL PROCESSES

Simulation of a Flow of a "Sedate" Reaction Mass in a Screw Reactor with a Thin Wall Layer

A. B. Golovanchikov, A. A. Shagarova, and N. A. Dul'kina

State Technical University, Volgograd, Russia

Received November 13, 2008

Abstract—A transition to a flow virtually non-gradient in a screw reactors of heavy sedate liquid with thin wall layer is considered. The graphs of the differential response functions of the known models based on the ideal gas law for structures of flows (ideal mixture, ideal displacement, laminar and turbulent flows) in comparison with the response function of the sedate reaction mass were presented. The flow structure corresponds to the regime of the ideal displacement in the screw reactor at a treatment of the sedate reaction mass when air, water or other thin liquid are fed as lubricant in the wall layer.

DOI: 10.1134/S1070427209040405

In many cases rheological properties of solutions and melts of polymers and reaction masses are described by a power rheological equation of Ostwald-de Waele with a relation between components of a stress tensor and a velocity of deformation looking as [1–3]

$$P_{ij} = 2k\left(\frac{1}{2}I_2\right)^{\frac{n-1}{2}} \times \dot{\varepsilon}_{ij}\,. \tag{1}$$

The possibility of the transfer to the practically non-gradient flow of the heavy sedate liquid in a pipe with thin wall layer when an anormality of the viscosity is simulated by equation (2)

$$\eta = k\left(\frac{1}{2}J_2\right)^{\frac{1-n}{2}}, \tag{2}$$

and in the case of a sample shift in the pipe it simulated by equation (3)

$$\eta = k\left(\frac{dV_r}{dz}\right)^{1-n}. \tag{3}$$

Analogous non-gradient profile of the velocity in the pipe of the heavy liquid with the thin wall layer was obtained for the Newtonian liquid flow [5, 6] at n = 1 and η = const whose properties were described by equation

$$\tau = \eta\,\dot{\gamma}. \tag{4}$$

It was shown in [2] that also at the flow of the heavy reaction mass in the screw reactor with the thin wall layer when the rheological properties are described by equation (4) the reaction mass moved practically in the non-gradient regime, and possessed the structure of the flow of the ideal displacement, while coils of the screw, and in particular, installed between them additional agitators provided the ideal mixture in a radial direction [8, 9].

Let us show that for heavy sedate reaction mass, with abnormal viscosity described by equation (2) that moves in the axial direction z and simultaneously rotates with the screw in the presence of the thin wall layer, the velocity profile V_z approaches the profile of the ideal displacement [10].

A scheme of the considered flow is presented in Fig. 1.

Due to the symmetry the partial derivatives of the velocity components with respect to φ equal to zero.

The velocity component V_r is absent. Only the derivatives dVz/dr and dV_φ/dr exist.

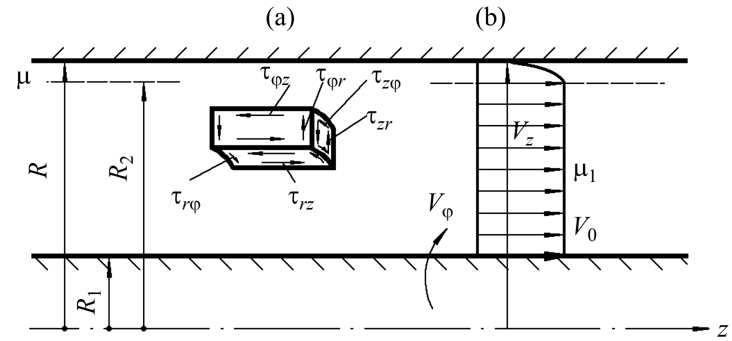

Fig. 1. The scheme of the axial movement of the sedate liquid with the thin wall layer (a) a diagram of the tangential stresses in the liquid elemenets, (b) velocity profile.

In this case for cylindrical coordinates we obtain

$$I_2 = 2\left(\frac{dV_\varphi}{dr} - \frac{V_\varphi}{r}\right)^2 + 2\left(\frac{dV_z}{dr}\right)^2, \tag{5}$$

$$\eta = k\left[\left(\frac{dV_\varphi}{dr} - \frac{V_\varphi}{r}\right)^2 + \left(\frac{dV_z}{dr}\right)^2\right]^{\frac{1-n}{2}}$$

We assume that owing to the above noted [4–7] that $dV_z/dr \to 0$ or

$$\left(\frac{dV_\varphi}{dr} - \frac{V_\varphi}{r}\right) \rangle\rangle \left(\frac{dV_z}{dr}\right), \tag{6}$$

then only the rotary movement of the reaction mass influences the effective viscosity:

$$\eta = k\left(\frac{dV_\varphi}{dr} - \frac{V_\varphi}{r}\right)^{1-n}, \tag{7}$$

And since $V_\varphi = \omega \cdot r$, then

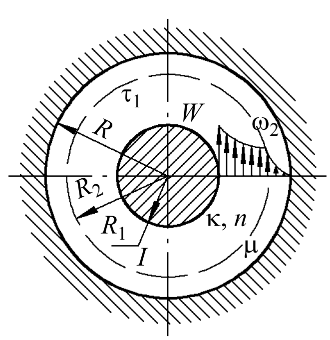

Fig. 2. The scheme of the rotary movement of the sedate liquid with thin wall layer.

$$\eta = k\left(r\frac{\partial\omega}{\partial r}\right)^{1-n} \tag{8}$$

From the equation of the movement in cylindrical coordinates [1] we obtain

$$\frac{d(r^2\tau_1)}{dr} = 0 \quad R_1 \le r \le R_2$$

A solution of the last equation does not depend on the rheological properties of the reaction mass and looks as

$$\tau_1 = \frac{C_1}{r^2} \quad R_1 \le r \le R_2 \tag{9}$$

Taking into account equation (8) for the sedate liquid we obtain

$$\tau_1 = k\,r\left(\frac{\partial\omega_1}{\partial r}\right)^n. \tag{10}$$

Equation (8) follows from a joint solution of equations (9) and (10) with boundary conditions $r=R_1$, ω_1=w

$$\omega_1 = w + C_1(r^{1-3/n} - R_1^{1-3/n}). \tag{11}$$

Close mathematical arrangements for the thin wall layer with boundary condition $r = R, \omega_2=0$ lead to equation (12)

$$\omega_2 = C\left(\frac{1}{r^2} - \frac{1}{R^2}\right). \tag{12}$$

For determination of integration constants C_1 and C in equation (11) and (12) we use conditions of the equality of the angular velocity and tangential stresses at $R = R_2$. Then at $\omega = \omega_1$

$$\begin{cases} \omega_1 = w + C_1\left(R_2^{1-3/n} - R_1^{1-3/n}\right) \\ \omega_2 = C\left(\dfrac{1}{R_2^2} - \dfrac{1}{R^2}\right). \end{cases} \tag{13}$$

Since from equation (11)

$$\frac{d\omega_1}{dr} = \frac{\left(1 - 3/n\right)C_1}{r^{3/n}} \tag{14}$$

and the velocity gradient V_φ equals to

$$\frac{dV_\varphi}{dr} = C_1\left(1 - 3/n\right)r^{1-3/n},$$
$$R_1 \le r \le R_2$$

from equation (12) we obtain $d\omega/dr = -2C/r^3$ and then

$$\begin{cases} \tau_1 = \tau_2 = -k\left[R_2 \dfrac{\left(1 - 3/n\right)C_1}{R_2^{3/n}}\right]^n \\ \tau = \tau_2 = \dfrac{2\mu R_2 C}{R_2^3}. \end{cases} \tag{15}$$

Equating the right items of the equations of sets (13) and (15) we get a set of two equations for calculation of the integration constants C_1 and C

$$\begin{cases} w + C_1\left(R_2^{1-3/n} - R_1^{1-3/n}\right) = C\left(\dfrac{1}{R_2^2} - \dfrac{1}{R^2}\right) \\ -k\left[R_2 \dfrac{\left(1 - 3/n\right)C_1}{R_2^{3/n}}\right]^n = \dfrac{2\mu R_2}{R_2^3} C \end{cases}. \tag{16}$$

As a result we have a transcendent equation to compute the constant C_1

$$a\, C_1^n = b - f\, C_1, \tag{17}$$

where $a = -k\, R_2^{n-1}\left(1 - \dfrac{3}{n}\right)^n \left(\dfrac{1}{R_2^2} - \dfrac{1}{R^2}\right)$,

$b = 2\mu R_2 W$;

$f = 2\mu R_2\left(R_1^{1-3/n} - R_2^{1-3/n}\right)$.

An algebraical expression for the integration constant C follows from the first equation of set (16):

$$C = \frac{w + C_1\left(R_2^{1-3/n} - R_1^{1-3/n}\right)}{\left(\dfrac{1}{R_2^2} - \dfrac{1}{R^2}\right)}. \tag{18}$$

The computed values of angular and linear velocities of the rotary movement of the sedate liquid with the thin wall layer were listed in Table 1 at $n = 0.6$; $k = 10$; $m = 10^{-3}$ Pa s; R = 0.15 m; $R^1 = 0.05$ m; $R^2 = 0.1485$ m, so a thickness of the wall layer of the thin liquid (water) was 1.5 mm or 1% from a body radius R; $w = 6.28$ s^{-1} (or a turn of the screw per second). The values of $C_1 = 5.03 \times 10^{-8}$; $C = 6.95$; $a = 44.46$; $b = 1.86 \times 10^{-3}$; $f = 47.57$.

As shown in Table 1 for the sedate liquid the angular velocity approaches the angular velocity of the screw rotation and all its changes from w to 0 occur in the wall layer of the thin liquid (water) of the thickness of 1.5 mm. From general differential equation of the movement in the stresses along the axis z we get [1]

$$\tau_{rz} = \frac{\Delta p}{2l} r + \frac{m}{r}, \tag{19}$$

where m is an integration constant.

For this complex flow within the channel of the screw reactor with the rotary and forward movement of the sedate liquid we take into account assumption (6) and equation (8) to get

$$\tau_{rz} = \left[k\left(r \frac{\partial \omega_1}{\partial r}\right)^{1-n}\right] \frac{dV_z}{dr} \tag{20}$$

or substituting the value of $\partial\omega_1/\partial r$ from equation (14) we can write

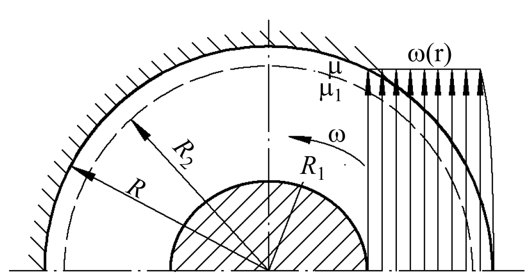

Fig. 3. Profile of the angular velocities of the sedate and thin wall liquid in the screw reactor.

Table 1. Dependence of the angular and linear velocities of the rotary movement of the sedate liquid with thin wall liquid

Thin wall layer $R_1 \le r \le R_2$			The thin wall liquid $R_2 \le r \le R$	
r_1, m $\times 10^2$	ω_1, s^{-1}	V_φ, m/s	r, m $\times 10^2$	ω, s^{-1}
5	6.28	0.314	14.85	6.27
5.985	6.275	0.375	14.865	5.63
6.97	6.274	0.437	14.88	5.0
7.955	6.273	0.499	14.895	4.37
8.94	6.272	0.561	14.91	3.74
9.925	6.272	0.622	14.925	3.11
10.91	6.272	0.684	14.94	2.491
11.89	5	6.272	0.746	14.955
12.88	6.272	0.808	14.97	1.23
13.865	6.272	0.869	14.985	0.062
14.85	6.272	0.931	15	0

$$\tau_{rz} = k\left[r\,\frac{(1-3/n)\,C_1}{r^{3/n}}\right]^{1-n}\frac{dV_{z1}}{dr},$$

$$R_1 \le r \le R_2, \tag{21}$$

$$\left\{\begin{aligned} m_1 &= k\left[(1-3/n)C_1\right]^{1-n} r^{\frac{5n-n^2-3}{n}}\frac{dV_{z1}}{dr} \\ m &= \mu r\,\frac{dV_z}{dr} \end{aligned}\right\}$$

for the viscous fluid in the wall layer

$$\tau_\mu = \mu\frac{dV_z}{dr} \quad R_2 \le r \le R \tag{22}$$

and for the stream without pressure drop in the opened screw reactor: $\Delta P/l \to 0$.

Then equation (21), and (22) taking into account equation (19) will look as

$$\begin{aligned} &R_1 \le r \le R_2, \\ &R_2 \le r \le R. \end{aligned} \tag{23}$$

A separation of variables and the integration of both equations of set (23) lead to the following equation

$$V_{z1} = \left\{\frac{m_1}{k\left[(1-3/n)C_1\right]^{1-n}}\right\}\left(1-\frac{5n-n^2-3}{n}\right) \times r^{\left(1-\frac{5n-n^2-3}{n}\right)} + p_1;$$

$$V_z = \frac{m}{\mu}\ln r + p,$$

Or reducing the factors attached to r, we can write

$$\begin{aligned} V_{z1} &= M_1 r^{\left(1-\frac{5n-n^2-3}{n}\right)} + p_1; \\ V_z &= M\ln r + p, \\ &R_1 \le r \le R_2, \\ &R_2 \le r \le R. \end{aligned} \tag{24}$$

The integration constant p_1 and p can be computed from the boundary conditions.

$$\begin{aligned} r &= R_1, \quad V_{z1} = V_0, \\ r &= R, \quad V_z = 0. \end{aligned}$$

Then

$$V_{z_1} = V_0 + M_1\left[r^{\left(1-\frac{5n-n^2-3}{n}\right)} - R_1^{\left(1-\frac{5n-n^2-3}{n}\right)}\right],$$

$$R_1 \le r \le R_2,$$

$$\begin{aligned} V_z &= M\ln\frac{r}{R}, \\ R_2 &\le r \le R. \end{aligned} \tag{25}$$

Conditions of an equation of the velocities and the tangential stresses ϕ_{rz} and ϕ_M on the boundary radius of both liquids R_2 can be used for computation of the integration constants M_1 and M. From equations (24) and (25) we obtain

$$M_1 = \frac{V_0(\mu/k)}{n_1\ln(R_2/R_1)\,[(3/n-1)C_1]^{1-n} + R_1^{n_1} - R_2^{n_1}};$$

$$M = \frac{V_0 + M_1(R_2^{n_1} - R_1^{n_1})}{\ln(R_2/R_1)}, \tag{26}$$

where $n_1 = 1 - (5n - 3 - n_2)/n$, and the velocity gradient *dVz1/dr* in the area of the sedate liquid stream $R_1 \le r \le R_2$ is calculated by equation, that we get from the first equation of set (24)

$$\frac{dV_{z1}}{dr} = M_1 n_1 r^{n_1-1}. \tag{27}$$

Results of the computations for the dependences of

Table 2. Dependence of velocities and velocity gradient on the radius

Sedate liquid $R_1 \le r \le R_2$				The thin wall liquid $R_2 \le r \le R$	
r_1, m $\times 10^2$	V_{zl}, m s^{-1}	$-V_{zl}/dr$, s$^{-1}\times 10^4$	$-V_1/dr$, s$^{-1}\times 10^4$	r_1, m $\times 10^2$	V_z, m s^{-1}
5	0.2	1.51	302.3	14.85	0.199
5.985	0.199	1.671	156.8	14.865	0.18
6.97	0.199	1.831	83.26	14.88	0.16
7.955	0.199	1.982	50.25	14.895	0.14
8.94	0.199	2.125	31.50	14.91	0.12
9.925	0.199	2.263	20.74	14.925	0.1
10.91	0.199	2.395	14.20	14.94	0.08
11.895	0.199	2.523	10.05	14.955	0.06
12.88	0.199	2.616	7.312	14.97	0.04
13.865	0.199	2.766	5.415	14.985	0.02
14.85	0.199	2.882	4.138	15	0

the velocities of the sedate liquid V_{z1} and the thin wall liquid V_z on the radius, and also analogous dependences for the velocity gradients dV_{z1}/dr and dV_z/dr calculated by equations (24) and (27) at $V_0 = 0.2$ m s^{-1} and $\omega = 2p\ (c - 1)$ are presented in Table 2. Values of $n_1 = 1.6$; $m_1 = -5.66 \times 10^{-4}$; $m = -19.9$.

As evident from Table 1 for the sedate liquid the velocity V_{z1} approaches constant, and all velocity changes occur in the wall layer, thereby the velocity gradient dV_{z1}/dr is significantly lesser than the gradient of a peripheral velocity of the sedate liquid dV_φ/dr, and both gradients tend to zero.

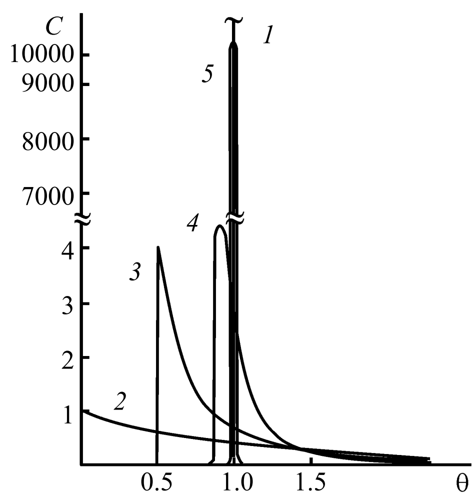

Fig. 4. Graphs of the response functions for the flow structures of (*1*) ideal displacement, (*2*) ideal mixture, (*3*) the laminar stream of the viscous liquid, (*4*) the turbulent flow in a pipe, (*5*) the sedate reaction mass with thin wall layer.

Therefore the assumption in equation (6) is right and the effective viscosity can be determined by equation (8) as depending only on the gradient of the angular velocity. Thus in the screw reactor treating the sedate reaction mass with consistency constant $k \times 10$ and flow indices $n \times 0.6$ the flow structure corresponds to the ideal displacement (Fig. 1b) when air, water or other thin liquid as a lubricant are fed in the wall layer. Since the consistency constant of the treated sedate reaction mass has an order $10^3 \le k \le 10^8$ [1, 3] then stream indices can be lesser than 0.6. For a dilatant sedate liquid $n > 1$ the assumption (6) is even more correct than for pseudoplastic liquid with the exponent lesser than unit.

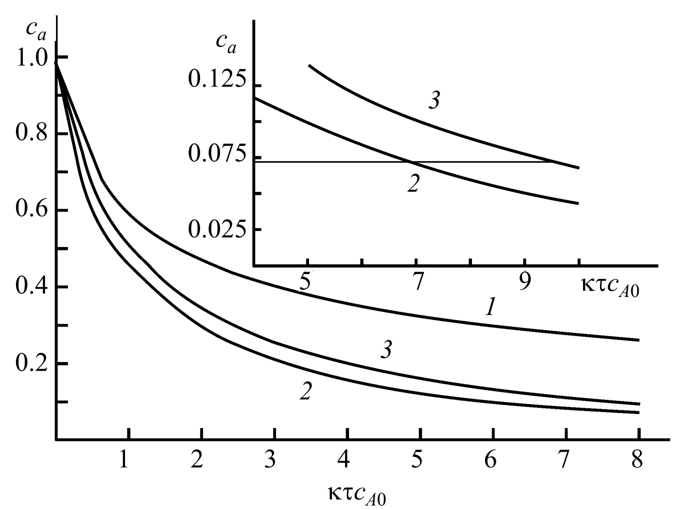

Fig. 5. Dependence od the relative concentration of component *A* for reaction $A+B \rightarrow R$ at $c_{B0}/c_{A0}=1.1$.

In the considered case the flow of the wall thin liquid is 0.5 $m^3 h^{-1}$ and is determined by integration of equation

$$dQ_\mu = 2 + \pi r V_z dr.$$

Taking into account the second equations of sets (25) and (26) we get:

$$Q_\mu = \frac{\pi\left[V_0 + M_1(R_2^{n_1} - R_1^{n_1})\right]}{\ln \frac{R_2}{R_w}} \times \left[\frac{R_2^2 - R_w^2}{2} + R_2^2 \ln\left(\frac{R_w}{R_2}\right)\right].$$

The flow of the sedate reaction mass is computed by analogous method according to equation

$$Q_1 = 2\pi\left[\begin{array}{c} V_0 - M_1 R_1^{n_1}\left(\frac{R_2^2 - R_1^2}{2}\right) + \\ \frac{M_1(R_2^{n_1+2} - R_1^{n_1+2})}{(n_1+2)} \end{array}\right]$$

and numerically equals to $Q_1 = 44.2\ m^3 h^{-1}$, thus the flow of the wall thin liquid is 1.3% relative to the flow of sedate reaction media for which the ideal displacement without a forced turbulization and large power consumptions is actual.

The differential response functions of the known models of the flow structures based on the model of ideal gas (ideal mixture, ideal displacement, laminar and turbulent flows) and the response function of the sedate reaction mass described by the first equation of set (13) are pictured on Fig. 4.

$$C = -\frac{2rV_{z1}^3}{(R_2^2 - R_1^2)V_{zc}^2(dV_{z_1}/dr)},$$

where $V_{zc} = Q_1/\pi(R_2^2 - R_1^2)$.

An analysis of the graphic dependences (Fig. 4) exhibits that the flow structure of the sedate reaction mass with thin wall layer (curve *5,* Fig .4) actually is close to the ideal displacement ($\delta(\theta - 1)$ is the Dirac function) described by line *1* on this graph. Even the turbulent structure of the flow that now we assume as the closest approach to the ideal displacement and described by function

$$C_T = 14\left[1 - (\theta_0/\theta)^7\right]\frac{\theta_0^7}{\theta^9};\ \theta > \theta_0 = \frac{98}{120}$$

significantly differs from the obtained structure of the flows in the screw reactor with the thin wall layer.

Even greater than the ideal displacement the laminar regime of the reaction mass in the pipe reactors (curve *3*, Fig. 4) that describes by a function

$$C_L = \frac{1}{2\theta^3};\quad \theta \ge 0.5.$$

The graphs of the dependence of relative final concentration of the component *A* on the parameter $\kappa_p \tau c_{A0}$ at $c_{b0} = c_{B0}/c_{A0}$ 1.1 for a simple chemical reaction $A + B \rightarrow R$ are presentedn Fig. 5.

The equations for the reactor computation for this reaction at various flow structures are known and look as [13, 14]

for reactor of the ideal mixture

$$C_c = \sqrt{\frac{1}{\kappa\tau c_{A0}} + \left[\frac{1 + \kappa\tau c_{A0}(c_{a0} - 1)}{2\kappa\tau c_{A0}}\right]^2} - \frac{1 + \kappa\tau c_{A0}(c_{b0} - 1)}{2\kappa\tau c_{A0}},$$

for reactor of the ideal displacement

$$C_d = \frac{c_{b0} - 1}{c_{b0}\exp[\kappa\tau c_{A0}(c_{b0} - 1) - 1]},$$

for reactor with the laminar flow

$$C_L = \int_{0.5}^{\infty} \frac{1}{2\theta^3}\left\{\frac{c_{b0} - 1}{c_{b0}\, exp\left[\kappa\tau c_{A0}\,(c_{b0} - 1)\theta\right] - 1}\right\} d\theta,$$

for reactor with the turbulent flow

$$C_T = \int_{\theta_0}^{\infty} 14\left[1 - \left(\frac{\theta_0}{\theta}\right)^7\right] \times \frac{\theta_0^7}{\theta^9}\left\{\frac{c_{b0} - 1}{c_{b0}\exp[\kappa\tau c_{A0}(c_{b0} - 1)\theta - 1]}\right\}\theta.$$

The graphs of last four equations are depicted on Fig. 5 (the graph of the turbulent flow practically coincides with the graph of the reactor of the ideal displacement).

As evident from the picture, the transition from laminar flow to turbulent flow makes possible the decrease in the reactor size 1.25 times at the conversion efficiency of 0.9 ($c_A = 0.1$). This difference in the volumes increases at the high conversion efficiency. Thus it is 42% at the conversion efficiency of 0.93, and 60% at 0.95.

NOTIFICATION

P_{ij} is the components of the stress tensor, Pa;

e_{ij} is the components of the tensor of the deformation velocities, s^{-1};

k is the consistency constant;

n is the flow index;

I_2 is quadric invariant of deviator of the tensor of the deformation velocities, s^{-2};

V_0 is longitudinal velocity of the reaction mass movement under the screw action, m s^{-1};

V_{zc} is an average velocity, m s^{-1};

u is dimensionless residence time;

c_{A0} and c_{B0} are the starting concentrations of the reaction components in the raw material;

κ_p is the constant of the reaction rate;

ϕ is an average residence time of the reaction mass in the reactor, s^{-1}.

REFERENCES

1. Torner, R.V., *Teoreticheskie osnovy pererabotki polimerov* (Theoretical Bases of Polymer Treatment), Moscow: Khimiya, 1977, 462 p.
2. Tyabin, N.V., *Reologicheskaya kibernetika* (Rheological Cybernetics), Volgograd: Volgogradskaya pravda, 1978.
3. Vinogradov, G.V., Malkin, A.Ya., *Reologiya polimerov* (Rheology Polymers), Moscow: Khimiya, 1977, 438 p.
4. Golovanchikov, A.B., Il'in, A.V., Il'ina L.A., *Izvestiya Volgogradskogo gosudarstvennogo tekhnicheskogo universiteta. Seriya: Kontseptual'noe proektirovanie v obrazovanii. Tekhnika i tekhnologii*, vol. 1, no. 5, 2004 pp. 19–21.
5. Golovanchikov, A.B. and Tyabin, N.V., *Matematicheskoe modelirovanie izobretenii v khimicheskoi tekhnologii. Uchebnoe posobie* (Mathematical Simulation of the Inventors in Chemical Technology), Volgograd, 1987.
6. Pivovarov, V.G., Tyabin, N.V., and Golovanchikov A.B., In *Reologiya, protsessy i apparaty khimicheskoi tekhnologii* (Reology, Processes and Apparatus in the Chemical Engineering), Volgograd: Volgogradskaya pravda, 1978, pp. 32–35.
7. Golovanchikov A.B., Shagarova A.A., Dul'kina, N.A., and Shandybina, I.M., *Khim. Prom*., 2007, vol. 84, no. 3, pp. 137–140.
8. RF Patent 2168351, 7 V01 F7/08 V01 J 19/18.
9. RF Patent 2314865, 7 V01 F7/08 V01 J, 19/18.
10. Golovanchikov, A.B., Shagarova, A.A., Dul'kina, N.A., and Dorodnikova, I.M., *Izvestiya Volgogradskogo gosudarstvennogo tekhnicheskogo universiteta. Seriya: Reologiya, protsessy i apparaty khimicheskoi tekhnologii,* vol 1, no. 11, 2007, pp. 8–9.
11. Middleman, S., *Flow of High Polymers*, Intersci., 1968.
12. Tyabin, N.V., *Metody kibernetiki v reologii i khimicheskoi tekhnologii: uchebnoe posobie* (Cybernetics in Rheology and Chemical Engineering: Textbook), Tyabin, N.V. and Golovanchikov, A.B., Volgograd: Volgogradskii politekhnichesii institut, 1983.
13. Kafarov, V.V., *Metody kibernetiki v khimii i khimicheskoi tekhnologii* (Cybernetics in Chemistry and Chemical Technology), Moscow: Khimiya, 1976.
14. Zakgeim, A.Yu., *Vvedenie v modelirovanie khimiko-tekhnologicheskikh protsessov* (Introduction in Modeling for Chemical Technological Processes), Moscow: Khimiya, 1973.