number of moles as a result of dissociation. In Eq. (26), the degree of dissociation of both first-order and second-order reactions is taken.

In addition, all the gas-dynamic functions include the quantities η, ω, ξ_{cr}, and R/μ, depending also on the degree of dissociation. The desired quantities are greatly influenced by the effective isobaric specific heat C_{pef}, which is high in dissociating gases. Then, it must be noted that the quantity $k_T - 1/k_T$ appearing in all the expressions for the gas-dynamic functions, according to Eq. (12), depends also on C_{pef}, R/μ, and ω.

Thus, these considerations indicate, with great reliability, that the thermophysical and chemical properties of dissociating gases have a great influence on the gas-dynamic functions obtained.

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TWO METHODS OF CALCULATING THE VELOCITY PROFILE OF A NON-NEWTONIAN LIQUID IN CYLINDRICAL CHANNELS OF ARBITRARY CROSS SECTION

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Two approaches to solving the problem of the flow of non-Newtonian liquid in cylindrical channels of arbitrary cross section are analyzed: variational and iterative approaches.

Formulation of the Problem

In the hydromechanis of non-Newtonian liquid, the problem of the velocity distribution in laminar steady flow in cylindrical singly connected channels of arbitrary cross section is known to be very interesting and of great practical importance.

The system of motion and continuity describing the given problem may be written in the form

$$\frac{\partial}{\partial \chi_1}\left(\mu(I_2)\frac{\partial V}{\partial \chi_1}\right)+\frac{\partial}{\partial \chi_2}\left(\mu(I_2)\frac{\partial V}{\partial \chi_2}\right)=-\frac{\partial P}{\partial z}=\text{const}, \tag{1}$$

$$\frac{\partial V}{\partial z}=0 \tag{2}$$

with the boundary condition

$$V|_\Gamma = 0, \tag{3}$$

where the second invariant of the deformation-rate tensor is

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$$I_2 = \left(\frac{\partial V}{\partial \chi_1}\right)^2 + \left(\frac{\partial V}{\partial \chi_2}\right)^2. \tag{4}$$

It is well known that an "explicit" solution of the problem in Eqs. (1)-(3) with an arbitrary general $\mu(I_2)$ does not exist. It is also known [1, 2] that the solution of the given problem, which consists in finding the real velocity field, is equivalent, on the basis of the law of mechanical-energy conservation, to determining the minimum of the functional

$$F(V) = \iint_\Omega d\chi_1 d\chi_2 \int_0^{I_2} \mu(\xi)\, d\xi + 2\frac{\partial P}{\partial z}\iint_\Omega V d\chi_1 d\chi_2. \tag{5}$$

Variational principles with subsequent numerical realization are usually used to find the function ensuring a minimum of the functional in Eq. (5). A brief analysis of the solution in the variational formulation follows.

Variational Method

In [3, 4], the problem in Eqs. (1)-(3) was considered for two regions: a rectangle and an ellipse. For a rectangular channel with sides $2a$ and 2b, the function realizing an extremeum of the functional in Eq. (5) is

$$V = (a^2 - \chi_1^2)(b^2 - \chi_2^2)(A_1 + A_2\chi_1^2 + A_3\chi_2^2 + \ldots + A_n\chi_1^{2x}\chi_2^{2y}), \tag{6}$$

and for an elliptical channel with axes $2a$ and 2b

$$V = \left(1 - \frac{\chi_1^2}{a^2} - \frac{\chi_2^2}{b^2}\right)(A_1 + A_2\chi_1^2 + A_3\chi_2^2 + \ldots + A_n\chi_1^{2x}\chi_2^{2y}). \tag{7}$$

The coefficients A_n are found from the condition of a minimum of the functional in Eq. (5) using the Ritz method

$$\frac{\partial F(V)}{\partial A_n} = 2\iint_\Omega \mu(I_2)\left(\frac{\partial V}{\partial \chi_1}\frac{\partial^2 V}{\partial \chi_1 \partial A_n} + \frac{\partial V}{\partial \chi_2}\frac{\partial^2 V}{\partial \chi_2 \partial A_n}\right) d\chi_1 d\chi_2 + 2\frac{\partial P}{\partial z}\iint_\Omega \frac{\partial V}{\partial A_n} d\chi_1 d\chi_2 = 0 \quad (n = 1,\ 2,\ \ldots,\ m). \tag{8}$$

After calculation of the integrand and the appropriate transformations, Eq. (8) is written in the form of a system of nonlinear equations in A_n, where, by analogy with [3, 4], m = 5 is assumed

$$\begin{aligned}
&A_1\Theta_{11} + A_2\Theta_{12} + A_3\Theta_{13} + A_4\Theta_{14} + A_5\Theta_{15} + \frac{\partial P}{\partial z}E_1 = 0,\\
&A_1\Theta_{21} + A_2\Theta_{22} + A_3\Theta_{23} + A_4\Theta_{24} + A_5\Theta_{25} + \frac{\partial P}{\partial z}E_2 = 0,\\
&A_1\Theta_{31} + A_2\Theta_{32} + A_3\Theta_{33} + A_4\Theta_{34} + A_5\Theta_{35} + \frac{\partial P}{\partial z}E_3 = 0,\\
&A_1\Theta_{41} + A_2\Theta_{42} + A_3\Theta_{43} + A_4\Theta_{44} + A_5\Theta_{45} + \frac{\partial P}{\partial z}E_4 = 0,\\
&A_1\Theta_{51} + A_2\Theta_{52} + A_3\Theta_{53} + A_4\Theta_{54} + A_5\Theta_{55} + \frac{\partial P}{\partial z}E_5 = 0.
\end{aligned} \tag{9}$$

Here

$$\Theta_{nm} = \iint_\Omega \mu(I_2)\,\varphi_{nm}(\chi_1,\ \chi_2)\, d\chi_1 d\chi_2; \quad E_n = \iint_\Omega \frac{\partial V}{\partial A_n} d\chi_1 d\chi_2;$$

$\varphi_{nm}(\chi_1, \chi_2)$ is the result of calculating the expression parentheses in the first integral in Eq. (8). After integration $\varphi_{nm}(\chi_1, \chi_2)$ and E_n will have a specific algebraic form for each region.

The system in Eq. (9) is solved by a Gaussian iterative method; repeated Gaussian quadrature is used to calculate θ_{nm}.

In contrast to [3, 4], the specific dependence chosen is the generalized Kutateladze–Khabakhpasheva rheological model [5] for a structurally viscous non-Newtonian liquid $d\varphi_* = -\varphi^n d\tau_*$ in the particular form

$$\varphi_* = \exp(-\tau_*), \tag{10}$$

where $\varphi_* = (\varphi_\infty - \varphi)/(\varphi_\infty - \varphi_0)$; $\tau_* = \theta(\tau - \tau_1)/(\varphi_\infty - \varphi_0)$; $\varphi = 1/\mu(I_2)$ is the viscosity of the liquid.

In realizing the variational approach, Eq. (9) is linearized in the first step of the calculation, by assigning some value $\mu^* = \text{const}$ to $\mu(I_2)$. Then A_n and V are determined in the first approximation. After calculating Eq. (4) and the effective viscosity from Eq. (10) or in the form of a power series [3, 4], θ_{nm} is again calculated. Thus, at each step of the calculation, Eq. (9) is linearized. It is completely obvious that, regardless of the form of rheological model, the Newtonian viscosity — usually μ_0 or correspondingly φ_0 — is specified as the first approximation. The velocity profile is Newtonian in the first step of the calculation. If the series of solutions of Eq. (9) then tends to some limit, this limit is the solution of Eq. (9) and of the problem.

Solution of Eqs. (1)-(3) in the variational formulation may be realized on a computer and has fair convergence. For example, in calculating a flow of model liquid obeying rheological Eq. (10) with the parameters $\theta = 0.1981$ $(\text{Pa}^2\cdot\text{sec})^{-1}$, $\varphi_0 = 1.9$ $(\text{Pa}\cdot\text{sec})^{-1}$, $\varphi_\infty = 13.7$ $(\text{Pa}\cdot\text{sec})^{-1}$, $\tau_1 = 0$ in a rectangular channel with sides $2a = 0.180$ m and $2b = 0.015$ m with $\partial P/\partial z = 600$ N/m^3, 40 iterations are required to reach a difference $|(A_n^k - A_n^{k-1})/A_n^k| = \varepsilon = 10^{-4}$.

The case of flow of the same model liquid with $\partial P/\partial z = 600$ N/m^3 in a semicircular channel with R = 0.006 m has also been considered. To reach the same error ε, 36 iterations are required. In view of the lack of symmetry with respect to the axis χ_1, the basis function is written in the form

$$V = (\chi_1^2 + \chi_2^2 - R^2)\chi_2(A_1 + A_2\chi_1^2 + A_3\chi_2 + A_4\chi_1^4 + A_5\chi_2^2 + A_6\chi_1^2\chi_2 + A_7\chi_1^2\chi_2^2 + A_8\chi_1^4\chi_2^2 + \ldots + A_n\chi_1^{2x}\chi_2^{y}). \tag{11}$$

A basic and very serious deficiency of the variational approach is the complexity of the choice of basis function for regions with partial symmetry — for example, semicircles — or no symmetry at all. For such regions, as a rule, it is possible to construct several variants of the basis function with subsequent testing by calculation. In addition, the total or partial lack of symmetry leads to increase in the number of equations in Eq. (9) (for a semicircle, the minimum set is m = 9).

A method of solving Eqs. (1)-(3) which is free from these deficiencies and converges as rapidly is proposed below.

Iterative Method

In [6] the approach suggested for solving Eqs. (1)-(3) was to replace the shear-stress components by the expressions

$$\mu(I_2)\frac{\partial V}{\partial \chi_1} = \frac{1}{2}\frac{\partial P}{\partial z}\frac{\partial U}{\partial \chi_1}, \quad \mu(I_2)\frac{\partial V}{\partial \chi_2} = \frac{1}{2}\frac{\partial P}{\partial z}\frac{\partial U}{\partial \chi_2}. \tag{12}$$

Substituting Eq. (12) into the initial nonlinear Eq. (1) gives a linearized result, in the form of the Poisson equation

$$\frac{\partial^2 U}{\partial \chi_1^2} + \frac{\partial^2 U}{\partial \chi_2^2} = -2, \tag{13}$$

by means of which, after substituting Eq. (12) into Eq. (10), an expression is found for determining the velocity field.

Since Eq. (13) describes the torsion of prismatic rods, the mathematical apparatus of torsion theory is used to find the velocity field in a prismatic channel.

It is obvious that reducing the initial Eq. (1) to Eq. (13) by means of Eq. (12) is correct in the case of flow of non-Newtonian liquid only for some symmetric regions: circles and strips. In other cases, this approach will describe the Newtonian velocity distribution [7].

In the proposed iterative approach, the substitution in Eq. (12) must be regarded as the first step of the iteration (the first approximation), in which the Newtonian viscosity $\mu^*(\chi_1, \chi_2)$ is calculated using the rheological model in Eq. (10) or any other. In this case, the shear stress in Eq. (10) will take the form

$$\tau = \frac{1}{2}\frac{\partial P}{\partial z}\sqrt{\left(\frac{\partial U}{\partial \chi_1}\right)^2 + \left(\frac{\partial U}{\partial \chi_2}\right)^2}. \tag{14}$$

Replacing the derivatives in Eq. (12) by difference analogs, the matrix V^1_{ij} describing a Newtonian velocity distribution is obtained in the first approximation

$$V^1_{ij}=\left(\frac{1}{2\mu^*(\chi_1,\ \chi_2)}\ \frac{\partial P}{\partial z}\sum_{\alpha=1}^{2}U'_{\chi_\alpha}+\frac{V^1_{i-1j}}{h_1}+\frac{V^1_{ij-1}}{h_2}\right)\frac{h_1h_2}{h_1+h_2}. \tag{15}$$

After calculating V^k_{ij} in the first step of the iteration (k = 1), $\mu^*(\chi_1, \chi_2)$ is again calculated using Eq. (10), in which the shear stress is determined as

$$\tau=\sqrt{\tau^2_{\chi_1}+\tau^2_{\chi_2}}=\mu^*(\chi_1,\ \chi_2)\sqrt{\left(\frac{\partial V^1}{\partial\chi_1}\right)^2+\left(\frac{\partial V^1}{\partial\chi_2}\right)^2}, \tag{16}$$

and in view of the implicit expression for the effective viscosity (consistency), the method of simple iteration is used to solve Eq. (10).

After calculating $\mu(I_2)$, like $\mu^*(\chi_1, \chi_2)$, in the first step of the iteration, Eq. (1) is written in the form

$$\frac{\partial}{\partial\chi_1}\left(\mu^*(\chi_1,\ \chi_2)\frac{\partial V}{a\chi_1}\right)+\frac{\partial}{\partial\chi_2}\left(\mu^*(\chi_1,\ \chi_2)\frac{\partial V}{\partial\chi_2}\right)=-\frac{\partial P}{\partial z},$$

or using difference operators

$$\Lambda_1Y+\Lambda_2Y=-\frac{\partial P}{\partial z}, \tag{17}$$

where $\Lambda_\alpha Y = (\mu^* Y_{\chi\alpha})_{\chi\alpha}$; α = 1, 2; $Y_{\gamma h}$ = 0.

The iterative scheme of the variable-direction method (BDM) [8] is used to solve Eq. (17); in the present case, it takes the form

$$\begin{gathered}\frac{Y^{k+1/2}-Y^k}{\tau^{(1)}}=\Lambda_1Y^{k+1/2}+\Lambda_2Y^k+\frac{\partial P}{\partial z},\\ \frac{Y^{k+1}-Y^{k+1/2}}{\tau^{(2)}}=\Lambda_1Y^{k+1/2}+\Lambda_2Y^{k+1}+\frac{\partial P}{\partial z}.\end{gathered} \tag{18}$$

Each equation of the system in Eq. (18) is solved by the fitting method [9]; for the first equation of the system, the fitting coefficients are calculated in the form

$$A^{k+1/2}_{ij}=\frac{\overset{*}{\mu}_{i+1j}+\overset{*}{\mu}_{ij}}{2h_1^2},$$

$$B^{k+1/2}_{ij}=\frac{\overset{*}{\mu}_{ij}+\overset{*}{\mu}_{i-1j}}{2h_1^2},$$

$$C^{k+1/2}_{ij}=\frac{1}{\tau^{(1)}}+\frac{\overset{*}{\mu}_{i+1j}+2\overset{*}{\mu}_{ij}+\overset{*}{\mu}_{i-1j}}{2h_1^2},$$

$$F^{k+1/2}_{ij}=\frac{\overset{*}{\mu}_{ij-1}+\overset{*}{\mu}_{ij}}{2h_2^2}Y^k_{ij-1}+\left(\frac{1}{\tau^{(1)}}-\frac{\overset{*}{\mu}_{ij+1}+2\overset{*}{\mu}_{ij}+\overset{*}{\mu}_{ij-1}}{2h_2^2}\right)Y^k_{ij}+\frac{\overset{*}{\mu}_{ij}+\overset{*}{\mu}_{ij+1}}{2h_2^2}Y^k_{ij+1}+\frac{\partial P}{\partial z},$$

and for the second equation in the form

$$A^{k+1}_{ij}=\frac{\overset{*}{\mu}_{ij}+\overset{*}{\mu}_{ij-1}}{2h_2^2},$$

$$B^{k+1}_{ij}=\frac{\overset{*}{\mu}_{ij+1}+\overset{*}{\mu}_{ij}}{2h_2^2},$$

$$C^{k+1}_{ij}=\frac{1}{\tau^{(2)}}+\frac{\overset{*}{\mu}_{ij+1}+2\overset{*}{\mu}_{ij}+\overset{*}{\mu}_{ij+1}}{2h_2^2},$$

$$F^{k+1}_{ij}=\frac{\overset{*}{\mu}_{ij}+\overset{*}{\mu}_{i-1j}}{2h_1^2}Y^{k+1/2}_{i-1j}+\left(\frac{1}{\tau^{(2)}}-\frac{\overset{*}{\mu}_{i+1j}+2\overset{*}{\mu}_{ij}+\overset{*}{\mu}_{i-1j}}{2h_1^2}\right)Y^{k+1/2}_{ij}+\frac{\overset{*}{\mu}_{i+1j}+\overset{*}{\mu}_{ij}}{2h_1^2}Y^{k+1/2}_{i+1j}+\frac{\partial P}{\partial z}.$$

The iterative parameters $\tau^{(1)}$ and $\tau^{(2)}$ are chosen so that the number of iterations is a minimum and is

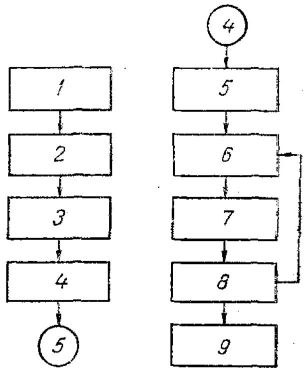

Fig. 1. Enlarged block diagram of the numerical solution of the problem in an iterative formulation: 1) specification of initial data; 2) calculation of the matrices $\partial U/\partial \chi_1$ and $\partial U/\partial \chi_2$; 3) calculation of τ from Eq. (14); 4) calculation of φ from Eq. (10); 5) calculation of V^1_{ij}; 6) calculation of φ from Eqs. (10) and (16); 7) solution of Eq. (17) by iterative VDM; 8) if $|(V^{k+1} - V^k)/V^k| < \varepsilon$, return to 6; otherwise, proceed to 9; 9) print matrices V, $\partial V/\partial \chi_1$, $\partial V/\partial \chi_2$.

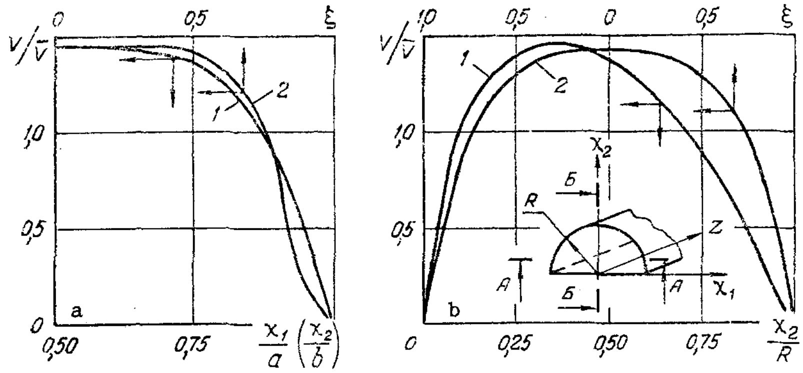

Fig. 2. Theoretical dimensionless velocity profiles: a) rectangular channel in a cross section with respect to the symmetry axis (1) and in a diagonal cross section (2); ξ is a dimensionless diagonal coordinate; b) semicircular channel in the radial cross section B—B (1) and in cross section A—A (2); ξ is the dimensionless coordinate in cross section A—A.

$$n(\varepsilon) \approx \frac{1}{\pi^2} \ln \frac{4}{\varepsilon} \ln \frac{4}{\eta},$$

where

$$\eta = \frac{1-t}{1+t}; \quad t = \sqrt{\frac{(\Delta_1 - \delta_1)(\Delta_2 - \delta_2)}{(\Delta_1 + \delta_2)(\Delta_2 + \delta_1)}}.$$

Here the boundaries δ_α, Δ_α of the operators Λ_α are

$$\delta_\alpha = \frac{4}{h_\alpha^2} \sin^2 \frac{\pi h_\alpha}{2 l_\alpha}, \quad \Delta_\alpha = \frac{4}{h_\alpha^2} \cos^2 \frac{\pi h_\alpha}{2 l_\alpha}, \quad \alpha = 1,\ 2, \quad \Omega (0 \leqslant \chi_\alpha \leqslant l_\alpha).$$

The formulas for determining the optimal values of the iterative parameters $\tau^{(1)}$ and $\tau^{(2)}$ were described in detail in [8].

After calculating $V^k(\chi_1, \chi_2)$ from Eqs. (17) and (18) in the second (k = 2) step of the iteration $\mu^*(\chi_1, \chi_2)$ is calculated again using Eq. (16). After determining $\mu^*(\chi_1, \chi_2)$ Eq. (17) is again realized. The process is repeated until $|(V^{k+1} - V^k)/V^k| = \varepsilon = \text{const}$. An enlarged block diagram of the solution is shown in Fig. 1.

This iterative process is analogous to that used in [10], where its convergence was investigated and proven.

Theoretical dimensionless velocity profiles with flow of the same non-Newtonian liquid in rectangular and semicircular channels are shown in Fig. 2. For a rectangular channel, U takes the form

$$U = \frac{32}{\pi^4} \sum_{m=1,3,\ldots}^{m} \sum_{n=1,3,\ldots}^{n} \frac{1}{nm\left(\frac{m^2}{a^2}+\frac{n^2}{b^2}\right)} \sin\frac{m\pi\chi_1}{a} \sin\frac{n\pi\chi_2}{b},$$

for a semicircular channel

$$U = -r^2 \sin^2\tilde{\varphi} + \sum_{n=1,3,5}^{n} b_n r^n \sin n\tilde{\varphi},$$

where

$$b_n = -\frac{8}{\pi}\,\frac{r^{2-n}}{n(n-2)(n+2)};\quad r = \sqrt{\chi_1^2+\chi_2^2};\quad \mathrm{tg}\,\tilde{\varphi} = \frac{\chi_1}{\chi_2}.$$

To solve the problem in an iterative formulation, 27 iterations are required for a rectangular region and 22 for a semicircle ($\varepsilon = 10^{-4}$).

For a rectangular channel, in addition to the cross section with respect to the symmetry axis, velocity profiles in a diagonal cross section are plotted, showing the presence and character of the "Stagnant" zones in the corners of the channel.

The velocity profiles in Fig. 2 are identical for the two methods.

The analysis of the calculation process shows that the form of the rheological model and the value of the axial pressure gradient — the free term in Eq. (18) — have no influence of the rate of convergence. For example, in solving the problem by the two methods but with a rheological model in the form of a power series [3], the same number of iterations is performed. However, the analysis also shows that the rate of convergence is influenced by the ratio φ_∞/φ_0; for a specific error ε, the number of iterations $n(\varepsilon)$ increases with increase in this ratio.

Thus, comparison of two methods of solving Eqs. (1)-(3) leads to the conclusion that the algorithm for numerical realization of the problem by the iterative method is less cumbersome that the variational algorithm and offers higher rates of convergence with less demand for computation time. This is associated with the obvious fact that finding the Newtonian velocity distribution in the first step of the iteration using the substitution in Eq. (12) is considerably simpler than solving Eq. (9).

But the basic advantage of the iterative method, in our view, is that there is no need to construct the basis function of the variational method, which is very complex for most regions. In contrast to the basis function, the function U is well known for practically any singly connected region from the theory of prismatic-rod torsion.

NOTATION

χ_1, χ_2, z, current coordinates; μ, effective viscosity of non-Newtonian liquid; I_2, second invariant of deformation-rate tensor; $\partial P/\partial z$, axial pressure gradient; V, flow rate; Ω, region with boundary Γ; a, b, half the sides of the rectangle or semiaxes of the ellipse; A_n, coefficients of the series; x, y, exponents; φ, consistency of non-Newtonian liquid; φ_0, φ_∞, consistency as $\tau \to 0$ and $\tau \to \infty$; τ, shear stress; τ_{χ_1}, τ_{χ_2}, components of shear stress; θ, τ_1, index and limit of stability of the macrostructure of the non-Newtonian liquid; k, number of iteration; ε, error of iterative process; R, radius of circle; U, auxiliary function, the solution of the Dirichlet problem for the Poisson equation; h_1, h_2, grid steps along the axes χ_1 and χ_2; γ_h, set of boundary grid points; Y, difference analog of the velocity V; Λ_α, difference analog of the derivatives; $\tau^{(1)}$, $\tau^{(2)}$. iterative parameters; A, B, C, F, fitting coefficients; $\bar{V}$, mean-flow-rate velocity of the flow; ξ, dimensionless coordinate in diagonal cross section, section A—A or x/a, y/b; i, j, numbers of difference-grid points; k + 1/2, intermediate iteration (subiteration); $n(\varepsilon)$, minimum number of iterations to reach the required error ε; δ_α, Δ_α, boundaries of the operators Λ_α; l_α, boundaries of the regions in the directions χ_1 and χ_2.