

tion of contaminants. The problem of petroleum gas use in minor power engineering should be solved by means of new, economically sound developments, which find wide application both in prolific and minor deposits of Tomsk region. Depending on ADG composition of

these deposits before power plants the following procedures should be carried out: separation from impurities and dehydration, purification from hydrogen sulfide and carbon dioxide, topping, removal of single heavy hydrocarbon gas constituents.

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## NUMERICAL INVESTIGATION OF CYLINDRICAL PRESS-MOULD FILLING PROCESS WITH POLYMER MASS BY THE MOLDING METHOD UNDER PRESSURE

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*On the basis of numerical solution of the problem on flow of nonlinear visco-plastic liquid with free surface the process of cylindrical press-mould filling has been studied. Mathematical statement of the problem is presented and the factors influencing the formation process are analysed. Numerical experiments carried out in the wide range of problem input parameters reveal the characteristics of hydrodynamic behaviour of free surface form of flowing polymer mass and demonstrate the influence of the main problem parameters on the basic characteristics of the process.*

#### Introduction

Qualitative and defectless manufacture of articles from polymeric materials (PM) by the molding method under pressure is mainly stipulated by structural-mechanical (rheological) properties of PM, operating mode of its recycling and constructive peculiarities of applied processing equipment. Therefore, both rheological characteristics of polymeric composition and the most important sides of the process itself should be deeply studied for formulating scientific requirements for manufacturing process.

Cylindrical press-moulds filling with polymeric mass by the molding method under pressure as well as by the method of free molding is characterized by one very important hydrodynamic feature – the presence of moving mass free surface contacting with solid stationary walls of a press-accessory. From this point of view, the whole process of press-moulds filling with polymeric mass is the process of formation and development of moving mass free surface up to its disappearance by the moment of cycle ending.

The experimental research [1, 2] shows that PM flow behavior in the elements of press-accessory is determined by a number of factors, which may be divided into three groups with a certain convention.

1. Hydrodynamic and rheological factors. Mass consumption in press-mould determined by processing equipment capacity, press-mould geometry; phys-

ical-mechanical mass properties (density, viscosity, rheological characteristics etc.); mass forces are referred to this group.

2. Thermalphysic factors. First of all, it is molding temperature conditions (temperature of inflowing polymeric mass, temperature and insulation properties of press-mould frame walls, temperature of environmental air) and thermalphysic properties of PM itself.
3. Physicochemical factors. The factors connected with hardening processes and finally determining time and manner of two previous groups of factors are usually referred to the third one.

The investigation of various factors influence on molding process of articles of PM is economically unprofitable directly in operation conditions. Therefore, it is necessary to use the methods of physical and mathematical simulation with further control and introduction of the obtained results into manufacturing. In mathematical simulation the simultaneous consideration of the whole complex of factors is rather difficult. In this connection, it is appropriate to simplify the problem relying on experimental data and considering the influence of the separate, most important factors from this point of view. The carried out investigations [3-9] show that the free surface form of moving mass in the elements of press-accessory is mainly defined by hydrodynamic and rheological parameters of processing mode of molding articles of PM.

### Mathematical problem statement

At the statement of mathematical problem the flow is considered to be laminar, isothermal and axisymmetric, and the typical time of hydrodynamic process is much more than relaxation time of moving polymeric mass stresses. In this case the system of equations describing the process of vertically disposed press-moulds filling with rheologically complex liquid in cylindrical coordinate system  $(z, r, \varphi)$ , using dimensionless variables, is written in the form [4]

$$\operatorname{Re} \left( \frac{\partial v_r}{\partial \tau} + \frac{1}{r} \frac{\partial (rv_r^2)}{\partial r} + \frac{\partial (v_r v_z)}{\partial z} \right) = -\frac{\partial p}{\partial r} + B \left( \nabla^2 v_r - \frac{v_r}{r^2} \right) + 2 \frac{\partial B}{\partial r} \frac{\partial v_r}{\partial r} + \frac{\partial B}{\partial z} \left( \frac{\partial v_r}{\partial z} + \frac{\partial v_z}{\partial r} \right), \quad (1)$$

$$\operatorname{Re} \left( \frac{\partial v_z}{\partial \tau} + \frac{1}{r} \frac{\partial (rv_r v_z)}{\partial r} + \frac{\partial v_z^2}{\partial z} \right) = -\frac{\partial p}{\partial z} + B \nabla^2 v_z + \frac{\partial B}{\partial r} \left( \frac{\partial v_r}{\partial z} + \frac{\partial v_z}{\partial r} \right) + 2 \frac{\partial B}{\partial z} \frac{\partial v_z}{\partial z} - \frac{\operatorname{Re}}{\operatorname{Fr}}, \quad (2)$$

$$\Delta p = -\operatorname{Re} \left( \frac{1}{r} \frac{\partial^2 (rv_r^2)}{\partial r^2} + \frac{2}{r} \frac{\partial^2 (rv_r v_z)}{\partial r \partial z} + \frac{\partial^2 v_z^2}{\partial z^2} \right) + 2 \frac{\partial B}{\partial r} \nabla^2 v_r + 2 \frac{\partial B}{\partial z} \nabla^2 v_z + 2 \frac{\partial^2 B}{\partial r^2} \frac{\partial v_r}{\partial r} + 2 \frac{\partial^2 B}{\partial r \partial z} \left( \frac{\partial v_r}{\partial z} + \frac{\partial v_z}{\partial r} \right) + 2 \frac{\partial^2 B}{\partial z^2} \frac{\partial v_z}{\partial z}. \quad (3)$$

In equations (1–3)  $\tau$  is the time;  $r, z$  are the axes of coordinates;  $v_r, v_z$  are the components of velocity vector corresponding to them;  $p$  is the pressure;  $\operatorname{Fr} = U^2/(gL)$  is the Froude number.

In accordance with the Schulman rheological model [10] the generalized Reynolds number ( $\operatorname{Re}$ ) and the liquid effective viscosity ( $B$ ) are determined in the form:

$$\operatorname{Re} = \rho U^{2-n/m} L^{n/m} / \mu^{n/m};$$

$$B = [\operatorname{Se}^{1/n} + I_2^{1/m}]^n / (I_2 + \varepsilon_0), \quad (4)$$

where  $\rho$  is liquid density;  $L$  is the tube radius  $R$  chosen as the typical linear dimension, in the case of round tube filling-up or the difference between the radius of outer cylinder  $R_2$  and inner one  $R_1$  at filling-up a pine-cylindrical type channel;  $\mu$  is the dynamic coefficient of liquid viscosity;  $U = Q/S$  is the average consumable velocity, determined through volumetric rate of liquid –  $Q$  and the area of channel section –  $S$ ; the dimensionless parameter of nonlinear viscoplasticity  $\operatorname{Se} = \tau_0 L^{n/m} / (U^{n/m} \cdot \mu^{n/m})$ , where  $\tau_0$  is the yield stress.

To write down the equations (1–3) the following variables are chosen as the dimensionless ones:

$$\bar{r} = \frac{r}{L}; \quad \bar{z} = \frac{z}{L}; \quad \bar{v}_z = \frac{v_z}{U}; \quad \bar{v}_r = \frac{v_r}{U}; \quad \bar{\tau} = \frac{\tau \cdot U}{L};$$

$$\bar{p} = (p - p_0) (L / (\mu U))^{n/m},$$

To have an opportunity for open-end scoring at calculation of viscoplastic fluid flows the small parameter

$\varepsilon_0$  is introduced into the expression for  $B$  in (4). Its value is chosen so that effective viscosity in the range of viscous flow  $\approx 10^{-4}$  is of the viscosity in the range of flow core ( $\varepsilon_0 = 0$ ) at solving the problems of nonlinear viscoplastic liquid dynamics.

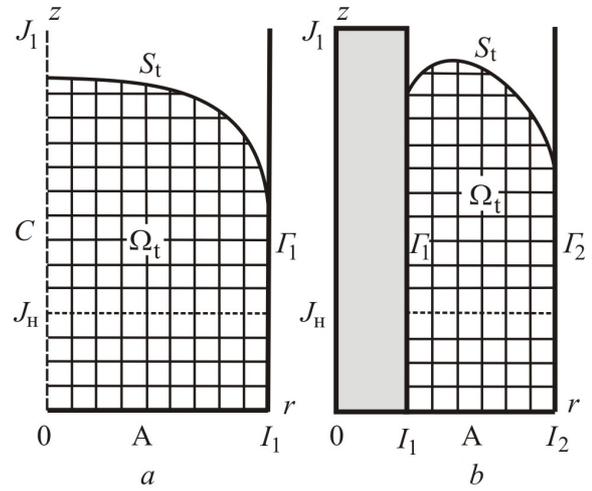
The expression for the intensity of strain rates  $I_2$  being a part of the second of ratios (4) may be presented as

$$I_2 = \sqrt{2 \left( \frac{\partial v_r}{\partial r} \right)^2 + 2 \left( \frac{v_r}{r} \right)^2 + \left( \frac{\partial v_z}{\partial z} \right)^2 + \left( \frac{\partial v_r}{\partial z} + \frac{\partial v_z}{\partial r} \right)^2}.$$

The initial and boundary conditions are also written in dimensionless form.

The free surface of mass  $S_t$  is supposed to be at the level  $J_H$  and to be flat at the moment of time  $t=0$  and at all fixed solid boundaries  $\Gamma_i$  ( $i=1, 2$ ) the adhesion condition is carried out.

$$v_z = v_r = 0. \quad (5)$$



**Fig. 1.** Boundaries of rated operating conditions: a) the round tube; b) the pine cylinders;  $z, r$  are the axes of coordinates;  $W_i$  is the rated operating conditions;  $S_t$  is the boundary of free surface;  $A$  is the input boundary;  $C$  is the axis of symmetry;  $\Gamma_i$  ( $i=1, 2$ ) are the fixed solid boundaries  $l_k, J_k$  are the numbers of nodes

At the input boundary  $A$  (Fig. 1) the velocity profile corresponding to stabilized flow of the given polymeric composition in the concerned channel is specified

$$v_z = f(r); \quad v_r = 0. \quad (6)$$

The form of the function  $f(r)$  in the expression (6) depends on rheological liquid properties and geometry of filled press-mould. The carried out numerical experiments showed that velocity profile (function  $f(r)$ ) specification at the input boundary in the form corresponding to the given liquid flow in the concerned channel does not influence greatly on the flow pattern in comparison with Newtonian velocity profile. It may be explained by the fact that the distance from the input boundary to the initial position of free surface exceeds the length of the initial hydrodynamic area. Therefore, in further calculations, the boundary conditions for the axial velocity component at the input boundary are

presented in the form:  $v_z=2(1-r^2)$  in the case of round tube filling-up and

$$v_z = \frac{2 \left( R_1^2 - r^2 + \frac{R_2^2 - R_1^2}{\ln(R_2/R_1)} \ln\left(\frac{r}{R_1}\right) \right)}{(R_2^2 + R_1^2 - (R_2^2 - R_1^2)/\ln(R_2/R_1))}$$

if the pine-cylindrical channel filling-up is considered and velocity radial component of the velocity  $v_r$  is supposed to be equal to zero in both cases [3].

In the case of round tube filling-up the conditions at the axis of symmetry  $C$  have the form

$$\frac{\partial v_z}{\partial r} = 0; \quad \frac{\partial p}{\partial r} = 0; \quad v_r = 0; \quad \frac{\partial B}{\partial r} = 0. \quad (7)$$

Two boundary conditions are specified on the free surface  $S_f$ : normal stress equation to pressure in the medium, adjacent with liquid, and condition of shearing stress absence. These conditions are written down in the local coordinate system  $(n, s, \theta)$ , connected with each point of free surface and have the form

$$p = 2B \frac{\partial u_n}{\partial n}; \quad \frac{\partial u_s}{\partial n} + \frac{\partial u_n}{\partial s} - \frac{u_s}{R_s} = 0, \quad (8)$$

where  $R_s$  is the radius of curvature of free surface.

The value of viscosity efficiency  $B$ , entering into the first of equations (8), is determined by the expression (4). Deformation rate intensity  $I_2$  in local orthogonal curvilinear coordinate system  $(n, s, \theta)$  may be presented in the form [3]

$$I_2 = \left[ 2 \left( \frac{\partial u_n}{\partial n} \right)^2 + 2 \left( \frac{v_r}{r} \right)^2 + 2 \left( \frac{\partial u_s}{\partial s} + \frac{u_n}{R_s} \right)^2 \right]^{\frac{1}{2}}.$$

Besides, the kinematic condition should be fulfilled on the free surface

$$\frac{dz}{dt} = v_z, \quad \frac{dr}{dt} = v_r.$$

Thus, to solve the assigned problem, the system consisting of two equations of motion in the directions  $r$  and  $z$ , the Poisson equation for pressure and equation connected effective viscosity with velocity field are used.

Numerical solution of the problem is found by the method of finite differences. For this purpose the given rated area  $\Omega_r$  (Fig. 1) is covered with the Euler chain of cells with the sizes  $h_1$  and  $h_2$  respectively in axial and radial directions. The method of difference analogues calculation of the initial system of differential equations using iterative schemes of the Liebmann type is stated rather detailed in papers [3, 4]. The original technique of boundary conditions realization on free surface in correct formulation is also described there.

For equivalence of boundary-value problem solution described by the equation system (1–4) with the corresponding initial and boundary conditions, consisting of continuity equation and equations (1, 2, 4, 9), carrying out the continuity equations at all the boundaries of rated area is required.

$$\frac{\partial v_z}{\partial z} + \frac{1}{r} \frac{\partial (rv_r)}{\partial r} = 0. \quad (9)$$

It ensures velocity field conservatism inside the area.

Thus, we obtain mathematical formulation of the problem on axial-symmetric flow of nonlinear viscoplastic liquid with free surface for describing the process of cylindrical press-moulds filling with polymeric mass.

### Results of calculation

Let us consider the vertical round tube and the channel of pine-cylindrical type filling with polymeric mass (Fig. 1).

On the basis of the method, stated in details in [3], the algorithm is developed and the calculation program of the process of cylindrical channels filling with rheologically complex liquid is constituted. The task of numerical investigation is the defining of the position and the form of free surface as well as finding velocity fields, pressure and press in nonlinear viscoplastic fluid flow.

The carried out calculations showed rather rapid convergence of iterative process (the number of iterations to convergence by  $\varepsilon=10^{-3}$  was in the range of 100–150) and stability of used difference scheme in wide range of input parameters change. The rheological constants  $n$ ,  $m$ , the parameter of nonlinear viscoplastic  $Se$  as well as criteria  $Re$ ,  $Fr$  were used as the input parameters at calculations of mentioned type flows. It was stated in papers [3–5], by means of dimensions analysis, that one of the main characteristics of the process is value  $W$ , being the ratio of  $Re/Fr$  ( $W=Re/Fr$ ), which is also similarity criteria as the combination of two criteria. Besides, it is necessary to note that in the case when the flow of nonlinear-viscous liquid is considered, i. e. the liquid without yield stress ( $Se=0$ ), the hydrodynamic pattern of the flow is determined by numbers  $Re$ ,  $Fr$  and parameters ratio  $n/m$ . When  $Se \neq 0$ , it is necessary to know the value of parameters ( $n$ ,  $m$ ) separately.

Let us consider some results of calculations.

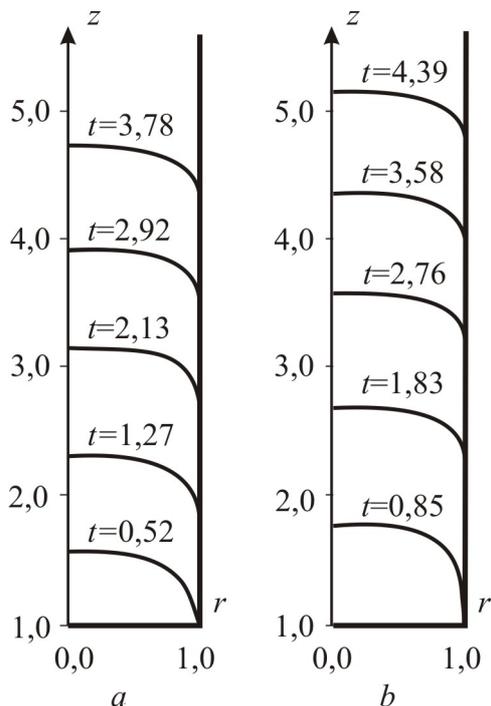
The development of free surface form and change of its position in time for two modes of cylindrical channel filling is shown in Fig. 2.

It is seen from the presented figure that the establishment of free surface form is observed when reaching the height equal approximately  $1,5D$  ( $D$  is the diameter of the channel). The comparison of cases *a*) and *b*) shows that  $W$  increasing results in moving mass front becoming flatter. The estimations carried out on the basis of metering characteristics analysis showed that the error in both case does not exceed 5 %.

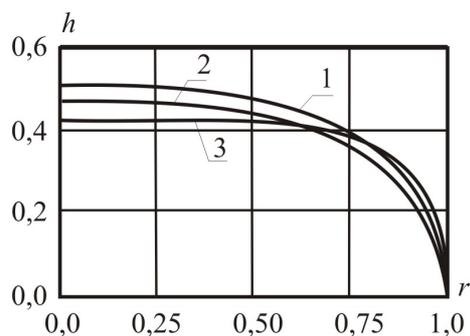
The influence of main hydrodynamic parameters on the established form of free surface is shown in Fig.

As it is seen from Fig. 3, at specified value of rheological constants  $n$  and  $m$  and parameter of nonlinear viscoplasticity  $Se$  the increase of  $W$  number results in the front of moving polymeric mass obtaining flatter form and value  $h_{max}$  determining maximal front rise, decreasing ( $h$  is the dimensionless quantity, equal to the difference between the moving coordinate  $z$  of free surface

and coordinate  $z$ , corresponding to the adherence point of free boundary to the channel wall).



**Fig. 2.** Change of position and form of free surface: a)  $Re=1,14 \cdot 10^{-5}$ ,  $Fr=1,52 \cdot 10^{-7}$ ,  $Se=0$ ,  $n/m=0,7$ ; b)  $Re=2,76 \cdot 10^{-4}$ ,  $Fr=9,52 \cdot 10^{-8}$ ,  $Se=8,12$ ,  $n=0,7$ ,  $m=1,0$



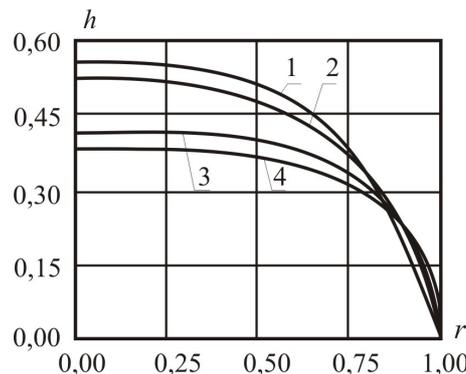
**Fig. 3.** The form of free surface depending on  $W$  at  $Se=0$ ;  $n/m=0,7$ : 1) 89,3; 2) 294; 3) 2330

The influence of parameter  $Se$  for two values of criterion  $W$  (curves 1, 2 and 3, 4) is shown in Fig. 4. The presented results show that at  $Se$  increasing the form of free surface also becomes flatter and at the same time the field of rod flow is rather visible. Besides, the results presented in the given figure illustrate once more the influence of parameter  $W$ .

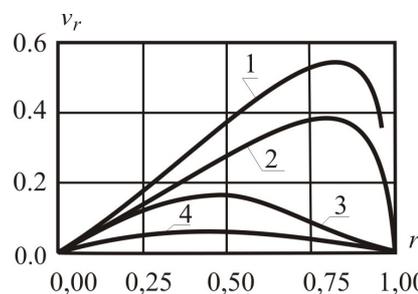
One of the peculiarities of liquid moving along free surface is the presence of two-dimensional flow zone. Intensive radial liquid flow is observed in this zone besides axial one. Therefore, it is supposed to be interesting to retrace the change of radial velocity in a front-line area and, thereby, to determine the boundaries of two-dimensional flow zone.

The distribution of radial constituent of the velocity vector plotted by its values in nodes of computational mesh be-

ing at different distances from free surface at  $Re=1,45 \cdot 10^{-6}$ ,  $Fr=1,62 \cdot 10^{-7}$ ,  $Se=0,6$ ,  $n=0,7$ ,  $m=1,0$ , is shown in Fig. 5.



**Fig. 4.** Influence of the parameter  $Se$  on the form of free surface: 1, 2)  $W=54,8$ ,  $n=1$ ,  $m=1$ ,  $Se=0,16$ ,  $Se=1,63$ , 3, 4)  $W=3330$ ,  $n=0,7$ ,  $m=1$ ,  $Se=1,89$ ,  $Se=143$



**Fig. 5.** Radial velocity distribution on channel section at different distance from free surface: 1)  $0,13D$ ; 2)  $0,26D$ ; 3)  $0,43D$ ; 4)  $0,6D$

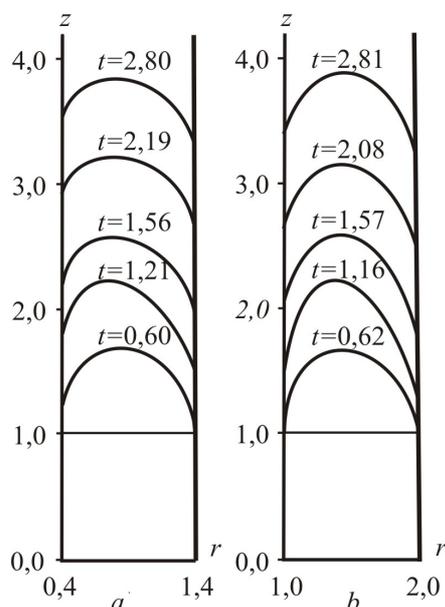
As it is seen from Fig. 5, radial velocity decreases when moving off the free surface and at a distance about  $0,7D$  the radial constituent of velocity is practically absent. This result allows for conclusion that at established mode the area of two-dimensional flow spreads over about  $0,7$  calibers from maximal front rise of fuel mass that conforms to the existing experimental data [1].

The calculation of the process of the channel of pine-cylindrical type filling gets rather sophisticated and requires more expenses of computer time in comparison with the round tube of the same length. The time of one variant calculation for a tube is, on average,  $1,5$  time less than in the given case. It is connected with the fact that at filling the channel of pine-cylindrical type the free surface of liquid has more complicated form and the number of iterations per one step increases in time.

At numerical investigation on the process of filling such channels along with rheological parameters and criteria considered in the previous paragraph it is necessary to take into consideration the ratio of radii of inner and outer cylinders  $R_2/R_1$ , which influences significantly the hydrodynamic pattern of the flow.

The change of position and form of free surface at filling of the channel of pine-cylindrical type for two modes of flow is shown in Fig. 6. It is seen from the presented figures that free surface form in both cases is established undergone certain transformation. The position of maximal front rise in these figures shows that

at increasing ratio  $R_2/R_1$ , the maximum shift to the inner cylinder in case a)  $R_2/R_1=3,5$ , and in the case b)  $R_2/R_1=2$  is observed.



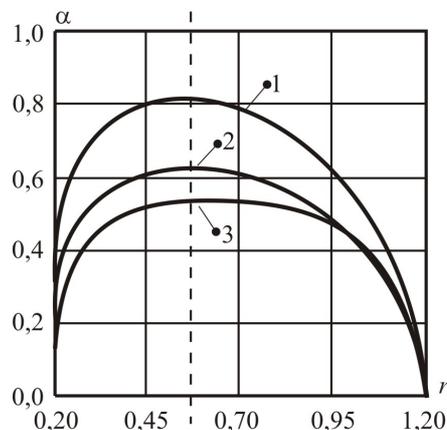
**Fig. 6.** Change of position and form of free surface: a)  $Re=1,79 \cdot 10^{-4}$ ,  $Fr=3,42 \cdot 10^{-7}$ ,  $Se=389$ ,  $n=0,7$ ,  $m=1,0$ ; b)  $Re=5,54 \cdot 10^{-5}$ ,  $Fr=6,16 \cdot 10^{-6}$ ,  $Se=0$ ,  $n/m=0,75$

The same result occurs at viscous liquid flowing in a gap between circular cylinders for axial velocity [11]. Besides, the behavior of free boundary in discussed cases indicates that when flowing in round tube, at increasing of  $W$  and  $Se$  criteria, liquid free surface becomes flatter.

Influence of these criteria on the form of free surface in the stated flow at fixed ratio of inner and outer cylinders radii ( $R_2/R_1=6$ ) and values of rheological parameters  $n$  and  $m$  is shown in Fig. 7

The analysis of the obtained results allows for conclusion that the position of the point defining maximal front rise does not depend on  $W$  and  $Se$  and completely determined by

the ratio  $R_2/R_1$ . The behavior of curves 1 and 2 shows that at the given value of the parameter  $Se$ , the increase of  $W$  results in free surface flattening and decreasing the distance between the points of adherence on the inner and outer lateral surface of cylinders. The growth of the parameter  $Se$  at fixed value  $W$  influences in the same way (curves 2, 3).



**Fig. 7.** Free surface form at  $R_2/R_1=6$ ;  $n=0,7$ ;  $m=1,0$ : 1)  $W=45,5$ ,  $Se=0$ ; 2)  $W=2,26 \cdot 10^4$ ,  $Se=0$ ; 3)  $Se=37,9$

## Conclusions

The numerical investigation on the process of bulky press-moulds filling by the method of molding under pressure has been carried out. The characteristics inherent to the studied process are considered. On the basis of the analysis of available experimental data it is shown that the rheological model suggested by Z.P. Shulman is the most acceptable from all angles for the investigation of flows of high-viscosity polymeric compositions. In terms of the developed numerical method the numerical solution of the problems on filling round tube and channel of pine-cylindrical type is obtained. The characteristics of flowing are discussed for each problem and the main results of calculation are presented. The influence of rheological parameters and flowing conditions on hydrodynamic pattern of the flow, free surface form, fields of velocity and pressure are stated.

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