Numerical simulation of the non-Newtonian fluid flow using the indirect boundary element method

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Abstract. The indirect boundary element method is formulated for a two-dimensional Stokes flow with the moving boundary when gravity force aids the flow. The governing equations of low Reynolds flow are formulated. The numerical technique is described. Two regimes of the fluid flow depending on the Stokes number value were detected: the regime of full filling and the jet flow regime. The comparison of obtained results with data of other authors is presented.

1. Introduction
The process of top-down filling of the vertical channel with non-Newtonian fluid is implemented during the injection molding of polymer melts. This kind of flow has several features. Firstly, the polymeric material flow in the channel is characterized by a moving free surface. Evolution of the free surface can cause formation of gas entrainment in the flow during the filling stage of the mold. This leads to a quality degradation of the finished product. Secondly, it is necessary to take into account the non-linear properties of polymer, i.e. to consider the non-Newtonian fluid flow. The behavior of the non-Newtonian fluid is dependent upon the viscosity variation within the flow domain. This leads to the nonlinear equations in the partial derivatives in contrast to the Stokes equations for the Newtonian fluid. In addition, polymeric materials have high viscosity that allows using the creeping flow model and does not consider the surface tension. The main focus is set on determination of the shape of the free surface which is especially important for manufacturing of polymer products [1-3].

The indirect boundary element method (IBEM) is now a well-established numerical technique which provides an efficient alternative to the prevailing finite difference and finite element methods for the solution of a wide range of engineering problems [4, 5]. Its basic idea consists of transformation of partial differential equations into equivalent boundary integral equations using the fundamental solution. In the present work, IBEM is used to simulate the non-Newtonian fluid flow in the vertical channel when gravity force aids the flow.

2. Governing equations
It is well known that non-Newtonian fluids do not behave as Newtonian fluids and that their viscosity is a nonlinear function of the shear rate. The viscosity of most non-Newtonian fluids is a decreasing function of the shear rate and this is known as shear-thinning behaviour. The non-Newtonian fluid behavior is described by the power law or Ostwald-de-Waele model:

\[
\tau_y = 2\eta \dot{\gamma},
\]

where \(\tau_y\) – the stress tensor deviator components, \(\eta = k\dot{\gamma}^{n-1}\) – the effective viscosity coefficient, \(k\) –
power law consistency, $n$ — the power law index, $\dot{\gamma} = \left(2\dot{\varepsilon}_{ij}\dot{\varepsilon}_{ij}\right)^{1/2}$ — deformation rate intensity, $\dot{\varepsilon}_{ij} = 1/2 \left(\partial u_i / \partial x_j + \partial u_j / \partial x_i\right)$ — components of the rate-of-strain tensor, $u_i$ — the velocity vector components, $x_i$ — the Cartesian coordinates.

The following scales are adopted for transition to dimensionless variables: for the coordinates — $L$ (a characteristic size of the domain occupied by the fluid), for the velocity — $U$ (characteristic flow velocity), for the pressure — $k(U/L)^n$. Equation (1) does not change the external view, but now $\eta = \dot{\gamma}^{n-1}$ is the dimensionless coefficient of effective viscosity.

The two-dimensional flow of the power law fluid at low Reynolds taking into account the gravity force is described by the dimensionless Stokes equations system:

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0, \ i, j = 1, 2,$$

where $\sigma_{ij} = -p_m \delta_{ij} + \tau_{ij}$ — stress tensor components, $p_m = \rho \text{St} x_2$ — modified pressure, $\rho$ — pressure, $\text{St} = \frac{\rho L^{n+1} \cdot (g \cdot e_2)}{U^n}$ — Stokes number, $e_2$ — unit vectors of the $x_2$ axis, $\delta_{ij}$ — the Kronecker delta. Equations (2) are used together with the continuity equation:

$$\frac{\partial u_i}{\partial x_i} = 0.$$

As a result, the flow is determined by two parameters — $\text{St}$, $n$, and also by the domain configuration if, of course, other forces are not considered in the boundary conditions, for example, the surface tension forces.

The formulation of the problem on filling a vertical channel with the non-Newtonian fluid is given in figure 1.

![Figure 1](image.png)

**Figure 1.** The solution domain ($S = S_1 + S_2 + S_3$).

The flow rate of the fluid at the inlet into the channel is considered to be given. The channel width is chosen as a characteristic length, the average flow velocity is characteristic velocity. The boundary
conditions at the inlet and on the solid walls are specified by the following relations:

\[
\begin{aligned}
u_t &= 0, \quad u_z(x_1) = \frac{2n+1}{n+1} \left( 1 - 2x_1^{\frac{n+1}{2}} \right), \\
u_t &= 0.
\end{aligned}
\] (4)

Dynamic and kinematic boundary conditions are performed on the free surface:

\[
t_i = \text{St}_i x_i n_i = t^N_i + \tau^{NN}_i n_j,
\] (5)

\[
dx_i = du_i,
\] (6)

where \(t^N_i\) – the linear part of the traction vector, \(\tau^{NN}_i\) – the nonlinear part of the stress tensor. The kinematic condition is written in the Lagrangian form and is used to find the shape of the free boundary. The initial condition is the shape of the free surface at the initial time.

3. Numerical solution

The indirect boundary element method is used for numerical solution. According to the postulates of the IBEM [6, 7], one can write down:

\[
\begin{aligned}
&u_i(x) = \int_S G_{ij}(x, \xi) \varphi_j(\xi) dS(\xi) + \int_\Omega G_{ij}(x, z) \Psi_j(z) d\Omega(z), \\
t^N_i(x) = \int_S F_{ij}(x, \xi) \varphi_j(\xi) dS(\xi) + \int_\Omega F_{ij}(x, z) \Psi_j(z) d\Omega(z),
\end{aligned}
\] (8)

where \(\varphi_j(\xi)\) – density of the fictitious sources distributed along boundary \(S\), \(\Psi_i(x)\) – density of the sources distributed about flow domain \(\Omega\). Functions \(G_{ij}\) and \(F_{ij}\) are the singular solutions of Stokes equations [8] and they are determined by formulas

\[
\begin{aligned}
&G_{ij}(x, \xi) = \frac{1}{4\pi} \left( \delta_{ij} \ln \frac{1}{r} + \frac{y_i y_j}{r^2} \right), \\
&F_{ij}(x, \xi) = \frac{y_i y_j y_{ij} n_i(x)}{\pi r^4},
\end{aligned}
\] (9)

where \(y_i = x_i - \xi_i\), \(r = y_i y_i^{1/2}\).

If the values of \(t^N_i(x)\), \(u_i(x)\) are specified on boundary \(S\), equations (8) make it possible to get the values of unknown boundary forces \(\varphi_j(\xi)\) (\(\xi \in S\)). But since \(\Psi_i(z)\) (\(z \in \Omega\)) functions were not known before, one can use an iteration method for this purpose.

For a numerical solution of equations (8), the constant elements and the constant internal cells are applied. The discretized boundary integral equations (8) acquire the following form:

\[
\begin{aligned}
&u_i(x^p) = \sum_{q=1}^{N} \phi^p_i \Delta G_{ij}^{pq} + \sum_{k} \sum_{m} \Psi_{jk}^{km} \Delta G_{ij}^{km}, \\
t^N_i(x^p) = \sum_{q=1}^{N} \phi^p_i \Delta F_{ij}^{pq} + \sum_{k} \sum_{m} \Psi_{jk}^{km} \Delta F_{ij}^{km},
\end{aligned}
\] (10)

where \(\Delta G_{ij}^{pq} = \int_{S} G_{ij}(x^p, \xi) dS(\xi)\), \(\Delta F_{ij}^{pq} = \int_{S} F_{ij}(x^p, \xi) dS(\xi)\), \(\Delta G_{ij}^{km} = \int_{\Omega} G_{ij}(x^p, z) d\Omega(z)\), \(\Delta F_{ij}^{km} = \int_{\Omega} F_{ij}(x^p, z) d\Omega(z)\), \(x^p\) is the middle of element \(p\), i.e. node \(p\). The coefficients of the obtained system of linear algebraic equations \(\Delta G_{ij}^{pq}\) and \(\Delta F_{ij}^{pq}\) for the case of the constant elements may be computed analytically [9].

To compute domain integrals \(\Delta G_{ij}^{km}\) and \(\Delta F_{ij}^{km}\), the standard quadrature Gaussian formulas are
used without the singularities extraction. During the process of computing, the quadrature formulas with 64 nodes are applied. The system of linear algebraic equations for the Newtonian fluid flow is solved by the Gauss standard method. In the case of non-Newtonian fluid flow, the algebraic equations system becomes nonlinear and is solved by simple iteration method. This method requires values of pseudo forces in each boundary element and each internal collocation point obtained from boundary conditions (for velocities and tractions) and the velocity field, found at the previous iteration. Internal cells sources are estimated numerically within a finite difference approach to velocity derivatives calculation.

4. Results
When filling the channel, the flow pattern of Newtonian and power law fluids is determined by parameters $St$ and $n$. Figures 2, 3 show the evolution of the free surface shapes of a Newtonian ($n = 1.0$) and shear-thinning fluids ($n = 0.9$ and 0.8).

There are two filling regimes. The change of the filling regimes occurs depending on the value of Stokes number. When $St = 1$, the fluid continuously flows and fills the channel. The initially flat free surface extends and takes the steady convex shape and moves along the channel. This regime is called the regime of fulfilling.

In figure 4, the comparison of a steady free surface shape, calculated in this paper, with results of [10] for case $n = 1.0$ is presented. We can see that the results are consistent.

![Figure 2. The evolution of the free surface shapes of a shear-thinning fluids: a − $n = 0.8$, $\Delta t = 0.2$, $n = 0.9$, $\Delta t = 0.2$](image-url)
Figure 3. The evolution of the free surface shapes of Newtonian fluid \( n = 1.0, \Delta t = 0.4 \)

Figure 4. The free surface shapes for \( n = 1.0, \text{St} = 0 \).

An increase of the value of Stokes number leads to formation of the jet flow regime. The free surface acquires the drop shape. With time, the minimum transverse size of jet decreases. In addition, we can see that power law index \( n \) also influences the free surface shape. With decreasing \( n \), the minimum transverse size increases.
In case $St = 5$ and $10$, the Newtonian fluid flow is characterized by jet deformation under the influence of gravity. In some time point the jet of fluid becomes unstable and flow symmetry is broken (figure 3). This leads to formation of voids which are classified in finished products as defects.

5. Conclusion

The presented results indicate that the indirect boundary element is an efficient means to solve the problems dealing with the non-Newtonian fluids with a free surface. The IBEM combined with the simple iteration method allows modelling the fluid flows at different power law index values. The governing equations were formulated and the numerical simulation method was described. The influence of flow non-linearity and the value of Stokes number on the shape free surface flow were considered. Two regimes of fluid flow were detected: the regime of fulfilling and the jet flow regime.

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