Modeling Die Swell of Second-Order Fluids Using Smoothed Particle Hydrodynamics

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1 Introduction

Polymeric materials have long been used for a variety of applications in our daily lives in the form of rods, tubes, and sheets. Most of these products are manufactured by extruding molten polymers (hereafter also referred to as a polymeric fluid, or liquid) through a die. In general, there are many steps in the manufacturing of polymeric products with desired shape and dimensions. These fabrication steps play a very important role in determining the quality of final products. The fabrication process starts with the synthesis of raw materials and ends with the manufacturing of finished products. The last processing step includes the extrusion of a polymeric fluid through a die. The extruded polymeric fluid exhibits viscoelastic characteristics because of the existence of normal stresses that can distort the cross section of the extrudate. The deformation of the polymeric liquid outside the die is widely referred to as the extrudate or the die swell. The die swell phenomenon leads to a change in the final shape of products. The extrudate swell is highly sensitive to rheological properties of polymers (whether being Newtonian or a non-Newtonian) and also the processing variables such as flow rate and temperature.

The die swell is defined as the ratio of the extrudate diameter to the die exit diameter. To improve both the quality of final products and the productivity of the fabrication process requires a good understanding of the rheological behavior of polymeric liquids, especially a thorough knowledge of the die swell phenomenon for controlling or reducing its undesired effect. This highly nonlinear and complex problem was the subject of extensive research in the last years. Toward this end, considerable effort has been dedicated toward predicting the behavior of the viscoelastic polymeric fluids using either experimental techniques [1,2] or numerical approaches. Numerical approaches reported in literature to model the die swell behavior include the finite element method [3–6], and finite difference technique [7] based on the marker and the cell philosophy [8,9]. Early works on the die swell can be classified into two- and three-dimensional models with various forms of die geometries such as two-dimensional convergent, divergent, or half converging/half tubular channels [3,4,6,8–10], and three-dimensional circular, square, or varied cross section channels [5,11]. These works have shown that the die swell is influenced by the rheological characteristic of polymeric fluids such as the sign and the value of first and second normal stress coefficients [6], process parameters such as the extrusion velocity [9], and the geometry of the die [1].

In all previously reported computational studies, the die swell process has been modeled using mesh-dependent approaches. When tackling problems that involve complex free surfaces, splashing, and fluid-solid interactions, mesh-dependent techniques, due to their Eulerian nature, require the solution of additional sets of equations for tracking free surface and may necessitate remeshing of computational grid in regions where large mesh-deformations and fractures may occur. Hence, modeling these types of flow problems with mesh-dependent methods presents significant challenges in computational fluid dynamics. Within the last two decades, meshless methods have started appearing in the field of computational fluid mechanics field as complementary methods to deal specifically with problems as
described above. Smoothed particle hydrodynamics (SPH) is one of the techniques in meshless Lagrangian particle methods used to solve partial differential equations. Although originally proposed to handle cosmological simulations [12], the SPH technique has become increasingly generalized to handle many types of fluid and solid mechanics problems such as heat transfer [13], multiphase flow [14], solidification [15], crystal growth [16], dynamic response of elastoplastic materials [17], free surface flows [18–20], and low-Reynolds number viscous flows [21]. Owing to its Lagrangian nature, the SPH technique offers noticeable advantages for modeling such flows in comparison to mesh-dependent methods. SPH advantages also include relatively ease of modeling complex material surface behavior, as well as relatively simple implementation of more complicated physics, such as non-Newtonian viscoelastic flows with and without free surface.

The SPH method has recently been extended to modeling non-Newtonian viscoelastic flows. The first attempt came with the work of Ellero et al. [22] in which a corotational Jaumann–Maxwell model was employed for studying the viscoelastic relaxation in a two-dimensional channel. The same first author also studied the transient flow between the parallel plates for both Oldroyd-B and upper-convected–Maxwell fluids at low Reynolds numbers [23]. The SPH method has also recently been used to model non-Newtonian flows with free surfaces. Shao and Lo [18] simulated a dam breaking problem with a modified version of cross-model. Fang et al. [19] studied the impact of a drop of an Oldroyd-B fluid on a rigid plate using a weakly compressible SPH (WCSPH) approach. Rafiee et al. [24] has also recently modeled bubble deformation in an Oldroyd-B shear flow and bubble rising in an Oldroyd-B fluid subjected to the combined effects of surface tension and buoyancy forces.

The motivation behind this work in particular is to scrutinize the feasibility and effectiveness of the SPH method to capture the extrude swell of a second-order viscoelastic non-Newtonian fluid. To be able to reveal that the developed SPH algorithm can also model the die swell of other types of polymeric fluids, a test simulation is also performed using the Oldroyd-B constitutive relation. To our best knowledge, the extrude swell problem has not been solved by the SPH or other meshless methods. Therefore, this work is a novel contribution to the field.

Having introduced the balance of mass and linear momentum as governing equations of the problem at hand along with various viscoelastic constitutive models in Sec. 2, the SPH method is presented along with the SPH discretization scheme for linearizing governing equations and the solution algorithms for the WCSPH approach in Sec. 3. In Sec. 4, the model problem together with its boundary conditions is outlined. In Sec. 5, three benchmark problems are solved to validate the WCSPH model used. Section 6 discusses the outcomes of the modeling studies in detail referring to the effect of various process and rheological parameters on the die swell. The paper concludes with some final remarks on the developed method and recapitulates important findings of the current work.

2 Governing Equations

The polymeric fluid is assumed to be a viscous incompressible non-Newtonian fluid with negligible thermal effects (i.e., isothermal flow). The governing equations used to solve the fluid problems in this article are the mass and linear momentum balance equations that are expressed in the Lagrangian form and given in direct notation as

\[ Dp/Dt = -p \nabla \cdot \mathbf{v}, \quad \rho D\mathbf{v}/Dt = \nabla \cdot \mathbf{\sigma} + \rho \mathbf{A} \cdot \mathbf{a} \quad (1) \]

The incompressibility condition requires that the divergence of the fluid velocity \( \nabla \cdot \mathbf{v} = 0 \) be zero. Here, \( \rho \) is the fluid density, \( \mathbf{v} \) is the divergence-free fluid velocity, \( \mathbf{\sigma} \) is the total stress tensor, and \( \mathbf{a} \) is the body force term, respectively. The total stress is defined as \( \mathbf{\sigma} = -p \mathbf{I} + \mathbf{T} \), where \( p \) is the absolute pressure, \( \mathbf{I} \) is the identity tensor, \( \mathbf{T} \) is the viscoelastic stress tensor. Finally, \( B/Dt \) is the material time derivative operator defined as \( D/Dt = d/dt + v \partial / \partial x \).

In the literature related to the die swell modeling of the second-order fluid, mainly two different forms of the constitutive equations have been used for the viscoelastic stress tensor, namely Rivlin–Ericksen [8,25,26] and Criminale–Ericksen–Filbey (CEF) [3–5,27] constitutive relations, which can be written, respectively, in direct notation as

\[ \mathbf{T} = \mu \mathbf{A} + z_1 \mathbf{A} + z_2 \mathbf{A} \cdot \mathbf{A} \quad (2) \]

\[ \mathbf{T} = \mu \mathbf{A} + 0.5z_1 \mathbf{A} - (0.5z_1 + z_2) \mathbf{A} \cdot \mathbf{A} \quad (3) \]

These two forms of the constitutive equations for the stress tensor can be represented in the following general form as \( \mathbf{T} = \mathbf{g} + \mathbf{g} \), where \( \mathbf{g} = \mu \mathbf{A} \) and \( \mathbf{g} \) represent in the given order the viscous and elastic components of the viscoelastic stress tensor. In some relevant literature, the viscoelastic stress tensor \( \mathbf{T} \) is also referred to as the extra stress tensor. Here, \( \mathbf{A} = \nabla \mathbf{v} + (\nabla \mathbf{v})^T \) and \( \mathbf{g} = \mathbf{g}/C_D \cdot \mathbf{D} \) are the deformation rate tensor and the kinematic tensor, respectively, where \( \mathbf{D}/C_D \) is a convected time derivative operator, \( \mu \) is the dynamic fluid viscosity, and \( z_1 \) and \( z_2 \) are the first and the second normal stress difference coefficients. The irreversible thermodynamic analysis on the second-order fluids performed by Massoudi, Vaidya, Dunn and Fosdick [25,28] requires the satisfaction of the following restrictions \( \mu > 0 \), \( z_1 > 0 \), and \( z_1 + z_2 = 0 \) so that all motions of the fluid are said to fulfill the Clausius–Duhem inequality. On the other hand, the experimental values of \( z_1 \) and \( z_2 \) for many non-Newtonian fluids that are assumed to obey constitutive relation given in Eq. (2) did not comply with the above given restriction, rather they satisfy the following conditions: \( \mu > 0 \), \( z_1 < 0 \), and \( z_1 + z_2 \neq 0 \), which we have used in our simulations. The material parameters \( z_1 \) and \( z_2 \) are functions of the magnitude of the deformation rate tensor. In what follows, the following definitions apply: \( N_1 = -z_1 A^{2}_{xy} \) and \( N_2 = z_2 A^{2}_{xy} \), where \( N_1 = T_{xx} - T_{yy} \) and \( N_2 = T_{yy} - T_{xx} \) are referred to as the first and second normal stress differences [5]. The second normal stress difference coefficient is difficult to measure and also considerably smaller than the first normal stress difference coefficient; hence, in many earlier works, it was either approximated through \( z_2 = -0.1 \times z_1 \) or neglected [3,8,27]. In the extrusion process, the second-order polymeric fluid can either swell or contract depending on the sign of the first normal stress difference coefficient.

When the viscoelastic polymeric liquid is deformed under the action of either stretching or shearing, or the combination of these two processes, the polymer molecules get stretched and entangled. If the polymer melt is exposed to a deformation for a short period of time, polymer molecules do remember their initial configuration, thereby being able to recover their initial shape. On the other hand, if the deformation is applied for an extended period of time, the polymer molecules tend to forget their initial positions and in turn cannot recover their original shape. This time-dependent phenomenon is known as the viscoelastic memory effect or the stress relaxation effect. The viscoelastic memory of polymeric materials is scaled with a dimensionless number referred to as Deborah number, \( DE = \lambda t \), which is defined as the ratio of the material relaxation time to the time scale of the flow (processing time). For die swell, the material relaxation time, defined as the time required for whole polymer molecules to relax and get used to its new state of deformation, can be formulated as \( \lambda = z_1/\mu \). The characteristic processing time \( t = l/v \) can be approximated as the ratio of the characteristic die diameter to the average speed of the flow through the die so that Deborah number can be reformulated as \( DE = z_1 \sqrt{\mu}/l \). Note that the polymeric liquid behaves as a
Table 1 Various forms of convected time derivatives that transform a tensor from convected to fixed coordinates, given in both direct and component notations

<table>
<thead>
<tr>
<th>Convected derivatives</th>
<th>Formulation</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Covariant form[25,26]</strong></td>
<td>(\mathbf{A}/\partial t = D\mathbf{A}/Dt + (\nabla \mathbf{v}) \cdot \mathbf{A} + \mathbf{A} \cdot (\nabla \mathbf{v})^T)</td>
</tr>
<tr>
<td>(\mathbf{A}/\partial t = D\mathbf{A}/Dt + \mathbf{v}<em>jA</em>{ij} + \mathbf{v}<em>jA</em>{ij})</td>
<td></td>
</tr>
<tr>
<td><strong>Contravariant form[8,9]</strong></td>
<td>(\mathbf{A}/\partial t = D\mathbf{A}/Dt - (\nabla \mathbf{v})^T \cdot \mathbf{A} - \mathbf{A} \cdot (\nabla \mathbf{v}))</td>
</tr>
<tr>
<td>(\mathbf{A}/\partial t = D\mathbf{A}/Dt - \mathbf{v}<em>jA</em>{ij} - \mathbf{v}<em>jA</em>{ij})</td>
<td></td>
</tr>
<tr>
<td><strong>Mixed covariant-contravariant form[5]</strong></td>
<td>(\mathbf{A}/\partial t = D\mathbf{A}/Dt + (\nabla \mathbf{v})^T \cdot \mathbf{A} - \mathbf{A} \cdot (\nabla \mathbf{v}))</td>
</tr>
<tr>
<td>(\mathbf{A}/\partial t = D\mathbf{A}/Dt - \mathbf{v}<em>jA</em>{ij} - \mathbf{v}<em>jA</em>{ij})</td>
<td></td>
</tr>
<tr>
<td><strong>Corotational (Jaumann) derivative[10]</strong></td>
<td>(\mathbf{A}/\partial t = D\mathbf{A}/Dt - \mathbf{v}<em>jA</em>{ij} - \mathbf{v}<em>jA</em>{ij})</td>
</tr>
<tr>
<td>(\mathbf{A}/\partial t = D\mathbf{A}/Dt - \mathbf{v}<em>jA</em>{ij} - \mathbf{v}<em>jA</em>{ij})</td>
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</table>

viscous fluid if the Deborah number goes to zero, while it acts as an elastic solid if De goes to infinity.

Our literature review on the die swell of a second-order fluid has also showed that there are different forms of convected time derivatives as given in Table 1. Convected time derivative is an operator that transforms a tensor from convected to fixed coordinates. There are no clear guidelines that can be followed to determine what form of time derivative might be the best or most appropriate for predicting the rheological behavior of polymeric fluids. Therefore, one should determine the usefulness of a given convected derivative based on its ability to predict the experimentally observed rheological behavior of polymeric fluids. In the following, for the sake of completeness, we present those that we have used in our simulation work to study their ability for predicting the die swell phenomenon correctly. The origin and the detailed derivations of these various forms of convected time derivatives can be found in Ref. \[29\].

The physical interpretation of the right-hand side of covariant, contravariant, and mixed covariant and contravariant convected time derivatives can be given such that the first term on the right-hand side represents the material time derivative of a tensor in the fixed coordinate systems, while the second and third terms represent the deformation (stretching) and rotational motions of a material element referred to in a fixed coordinate system as the velocity gradient tensor \(\mathbf{v}_{ij}\) (and \(\mathbf{v}_{ij}\)) can be expressed by the sum of deformation rate tensor \(d_{ij} = 0.5(\mathbf{v}_{ij} + \mathbf{v}_{ji})\) and the vorticity tensor \(\omega_{ij} = 0.5(\mathbf{v}_{ij} - \mathbf{v}_{ji})\). The Jaumann convected time derivative can be formed by adding covariant and contravariant convected time derivatives and then noting that \(\mathbf{v}_{ij} = d_{ij} + \omega_{ij}\). The second and third terms on the right-hand side of Jaumann derivative describe the rotational motion of the material element.

For the sake of completeness of the current work, we have also considered the die swell behavior of an Oldroyd-B fluid for which the constitutive equation is given by

\[
\mathbf{T} = \mu \mathbf{A} - \lambda_1 \varepsilon
\]

where \(\varepsilon = \mathbf{T} - \mu (\lambda_2/\lambda_1) \mathbf{A}\) that can also be written as \(\varepsilon = \varepsilon + \lambda_1 \varepsilon\), which upon casting into Eq. (4) produces the relation

\[
\varepsilon + \lambda_1 \varepsilon = \mu (1 - \lambda_2/\lambda_1) \mathbf{A}
\]

where \(\varepsilon\) represents the non-Newtonian part of the extra stress tensor. Here, \(\lambda_1\) and \(\lambda_2\) are the time constants of relaxation and retardation, respectively. It should be noted that for the Oldroyd-B fluid, the convariant form of the convected time derivative operator is used. Therefore, one can write the following relation from Eq. (5):

\[
e^{jk}(n+1) = (1 - \Delta t/\lambda_1) e^{jk}(n) + \Delta v_{ij} e^{ik}(n) + \Delta v_{jk} e^{j}(n) + (\mu_0 \Delta t/\lambda_1) (1 - \lambda_2/\lambda_1)(v_{ij} + v_{ji})
\]

where \(n\) is the temporal index.

3 Smoothed Particle Hydrodynamics

Smoothed particle hydrodynamics (SPH) is one of the members of meshless Lagrangian particle methods used to solve partial differential equations widely encountered in scientific and engineering problems. Unlike Eulerian (mesh-dependent) computational techniques such as finite difference, finite volume, and finite element methods, SPH does not require a grid as field derivatives are approximated analytically using a kernel function. In this technique, the continuum or the global computational domain is represented by a set of discrete particles. Here, it should be noted that the term particle refers to a macroscopic part (geometric position) in the continuum. Each particle carries mass, momentum, energy, and other relevant hydrodynamic properties. These sets of particles are able to describe the physical behavior of the continuum and also have the ability to move under the influence of the internal/external forces applied due to the Lagrangian nature of SPH \[30,31\].

For the clarity of the presentation, it is worthy of introducing notational conventions to be used throughout this article. All vector quantities are written either using index notation with Latin indices denoting the components or direct notations with lowercase boldface letters. These components will be written either as subscripts (when particle identifiers are not used) or superscripts (when particle identifiers are used). As well, throughout this article the Einstein summation convention is employed, where any repeated component index is summed over the range of the index. These superscripts do not represent any covariant or contravariant nature. Latin boldface indices (i, j) will be used as particle identifiers to denote particles and will always be placed as subscripts that are not summed, unless used with a summation symbol. For example, the position vector for particle i is \(\mathbf{r}_i = x_i \mathbf{e}_i\) where \(x_i\) components of the position vector and \(\mathbf{e}_i\) is a base vector. The distance vector between a pair of particles is indicated by \(\mathbf{r}_{ij} = \mathbf{r}_i - \mathbf{r}_j = (x_i - x_j) \mathbf{e}_i = r_{ij} \mathbf{e}_i\), and the magnitude of the distance vector \(r_{ij}\) is denoted by \(r_{ij}\).

The three-dimensional Dirac-delta function \(\delta^3(\mathbf{r}_{ij})\), also referred to as a unit pulse function, is the starting point of the SPH approximation technique. This function satisfies the identity

\[
f(\mathbf{r}_{ij}) = \int_{\Omega} f(\mathbf{r}) \delta^3(\mathbf{r}_{ij}) d^3\mathbf{r}_{ij}
\]
where $d^3 r_i$ is a differential volume element and $\Omega$ represents the total bounded volume of the domain.

The SPH approach assumes that fields of a given particle are affected by those of all other particles within the global domain. The interactions among the particles within the global domain are achieved through a compactly supported, normalized and even weighting function (smoothing kernel function) $W(r_{ij}, \kappa)$ with a smoothing radius $\kappa h$ (cut off distance, localized domain) beyond which the function is zero. Hence, in computations, a given particle interacts with only its nearest neighbors contained in this localized domain. Here, the length $h$ defines the support domain of the particle of interest and $\kappa$ is a coefficient associated with the particular kernel function. If the Dirac-delta function in Eq. (7) is replaced by a kernel function $W(r_{ij}, \kappa)$, the integral estimate or the kernel approximation to an arbitrary function $f(\vec{r}_i)$ can be introduced as

$$f(\vec{r}_i) \cong \langle f(\vec{r}_i) \rangle \equiv \int_{\Omega} f(\vec{r}_i) W(r_{ij}, \kappa) d^3 r_j$$

(8)

where the angle bracket $\langle \rangle$ denotes the kernel approximation, and $\vec{r}_i$ is the position vector defining the center point of the kernel function.

Approximation to the Dirac-delta function by a smoothing kernel function is the origin of the SPH method. The Dirac-delta function can be replaced by a smoothing kernel function provided that the smoothing kernel satisfies the following conditions [32]; namely, (a) normalization condition: the area under the smoothing function must be unity over its support domain, \[ \int \frac{W(r_{ij}, \kappa)}{d^3 r_j} = 1, \] (b) the Dirac-delta function property: as the smoothing length approaches to zero, the Dirac-delta function should be recovered $\lim_{\kappa \to 0} W(r_{ij}, \kappa) = \delta^3(r_{ij})$, (c) compactness or compact support that necessitates that the kernel function be zero beyond its compact support domain, $W(r_{ij}, \kappa) = 0$ when $r_{ij} > \kappa h$, (d) the kernel function is to be spherically symmetric even function, $W(r_{ij}, \kappa) = W(-r_{ij}, \kappa)$, and (e) the smoothing function should be positive within the support domain, $W(r_{ij}, \kappa) > 0$ when $r_{ij} < \kappa h$. Finally, the value of the smoothing function should decay with increasing distance away from the center particle. In literature, it is possible to find a wide variety of kernel functions that satisfy the above-listed conditions, such as Gaussian, cubic, or quintic kernel functions. The smoothing kernels can be considered as discretization schemes in mesh-dependent techniques such as finite difference and volume. The stability, the accuracy, and the speed of SPH simulation heavily depend on the choice of the smoothing kernel function as well as the smoothing length.

Throughout the present simulations, the compactly supported two-dimensional quintic spline kernel is used:

$$W(r_{ij}, \kappa) = \frac{7}{478 \pi h^3} \left\{ \begin{array}{ll} (3 - s_j)^5 - 6(2 - s_j)^5 + 15(1 - s_j)^5 & \text{if } 0 \leq s_j < 1 \\ (3 - s_j)^5 - 6(2 - s_j)^5 & \text{if } 1 \leq s_j < 2 \\ (3 - s_j)^5 & \text{if } 2 \leq s_j < 3 \\ 0 & \text{if } s_j \geq 3 \end{array} \right. \quad (9)$$

where $s_j = r_{ij}/h$. The spatial resolution of SPH is affected by the smoothing length. Hence, depending on the problem to be solved, each particle can be assigned to a different value of smoothing length. For a variable smoothing length, it is probable to violate Newton’s third law. For example, it might be possible for a particle $j$ to exert a force on particle $i$ and not to experience an equal and opposite reaction force from particle $i$. To ensure that Newton’s third law is not violated and the pairwise interaction among particles moving close to each other is achieved, the smoothing length is substituted by its average, defined as $h_0 = 0.5 (h_i + h_j)$. The averaged smoothing length ensures that particle $i$ is within the influence domain of particle $j$ and vice versa.

### 3.1 Spatial Derivatives and Particle Approximation in SPH

The SPH approximation for the gradient of an arbitrary function (i.e., scalar, vectorial, or tensorial) can be written through the substitution $f(\vec{r}_i) \to \partial f(\vec{r}_i)/\partial \xi^j$ in Eq. (8) to produce

$$\frac{\partial f(\vec{r}_i)}{\partial \xi^j} \cong \frac{\partial \{f(\vec{r}_i)\}}{\partial \xi^j} \equiv \int_{\Omega} \frac{\partial f(\vec{r}_i)}{\partial \xi^j} W(r_{ij}, \kappa) d^3 r_j$$

(10)

Upon integrating the right-hand side of Eq. (10) by parts and then using the Green–Gauss theorem, one can write

$$\int f(\vec{r}_i) W(r_{ij}, \kappa) d^3 r_j - \int f(\vec{r}_i) \frac{\partial W(r_{ij}, \kappa)}{\partial \xi^j} d^3 r_j$$

(11)

Here, the first term in Eq. (11) is referred to a boundary residual integral. Upon using the compactness property of the kernel function, which requires that the boundary residual integral be zero as well as noting that $\partial W(r_{ij}, \kappa)/\partial \xi^j = -\partial W(r_{ij}, \kappa)/\partial x^j$ for a constant smoothing length $h$, it can be shown that

$$\frac{\partial f(\vec{r}_i)}{\partial \xi^j} \cong \left\langle \frac{\partial f(\vec{r}_i)}{\partial \xi^j} \right\rangle \equiv \int_{\Omega} \frac{\partial f(\vec{r}_i)}{\partial \xi^j} \frac{\partial W(r_{ij}, \kappa)}{\partial \xi^j} d^3 r_j$$

(12)

The SPH approximation used for the gradient of a vector-valued function $f^p(\vec{r}_i)$ is an obvious extension of Eq. (12) and is obtained by replacing $f(\vec{r}_i) \to f^p(\vec{r}_i)$. Using a Taylor series expansion and the properties of a second-rank isotropic tensor, the SPH approximation for the gradient of a vector-valued function can also be introduced as

$$\frac{\partial^p f(\vec{r}_i)}{\partial \xi^j} = \int \left( f^p(\vec{r}_i) - f^p(\vec{r}_i) \right) \frac{\partial W(r_{ij}, \kappa)}{\partial \xi^j} d^3 r_j$$

(13)

In the above equations, the SPH approximations are written for a continuous distribution. If, however, we recognize that these integrations will be carried out over all $N$ discrete particles within the domain, the discrete SPH particle approximation can be obtained by replacing the integration with summation over particle $j$ to produce the SPH approximation of a field property $f^p(\vec{r}_i)$ at particle $i$ in terms of all other interacting particles $j$ and representing the particle volume as the ratio of a particle mass $m_j$ and particle density $\rho_j$. There are other alternative forms for the SPH gradient approximation of an arbitrary function. One that is also used within the context of this presentation can be formulated through using the product rule of differentiation on $\partial f^p(\vec{r}_i)/\partial \xi^j$ in combination with Eq. (12). In what follows, one can write
Similar to the derivation of Eq. (13), upon using a Taylor series expansion and the properties of second- and fourth-rank isotropic tensors, a general form of the SPH approximation for the second-order derivative of a vector-valued function $\frac{\partial^2 f}{\partial t^2}(\mathbf{r}_i)$ can be constructed [33,34] as

$$\frac{\partial^2 f}{\partial t^2}(\mathbf{r}_i) = \sum_{j=1}^{N} \frac{m_j}{\rho_j} \left( f^o(\mathbf{r}_j) - f^o(\mathbf{r}_i) \right) \frac{1}{r_{ij}} \left( \frac{4r_{ij}^3}{r_{ij}^2} - \delta_{ij} \right) \frac{\partial W(r_{ij}, h)}{\partial r_{ij}}$$

(15)

where $\delta_{ij}$ is the Kronecker-delta. The approximation for the Laplacian coming by contracting on indices $k$ and $l$ in Eq. (15) to produce

$$\frac{\partial^2 f^o}{\partial t^2} = \sum_{j=1}^{N} \frac{m_j}{\rho_j} \left( f^o(\mathbf{r}_j) - f^o(\mathbf{r}_i) \right) \frac{1}{r_{ij}} \frac{\partial W(r_{ij}, h)}{\partial r_{ij}}$$

(16)

### 3.2 SPH Solution Algorithms

There are two common approaches utilized in the SPH literature for solving the balance of the linear momentum equation. The first one is widely referred to as the weakly compressible SPH (WCSPH) wherein the artificial equation of state is implemented. The second approach, known as incompressible SPH (ISPH), the pressure is computed by means of solving a pressure Poisson equation. In this work, we have implemented the WCSPH approach. The artificial equation of state used in the WCSPH approach has the form of,

$$p - p_o = c_i^2(p - p_o)$$

where $p, p_o$ and $c_i$ are the pressure, reference pressure, and the speed of sound of the real fluid density, respectively. Upon selecting the sound speed $c_i$ such that

$$c_i \approx \sqrt{\frac{\mu}{\rho_o} L_o}$$

(17)

where $\mu$ is the viscosity, $\rho_o$ is the bulk density, $L_o$ is a characteristic length, and $c_i$ is the characteristic pressure change thereby preventing the dilatation of the fluid. The speed of sound $c_i$ for each particle must be chosen carefully to ensure that the fluid is very closely incompressible. It has been suggested by Morris et al. [21], that the square of the sound speed be chosen such that

$$c_i^2 \approx \varphi \max \left( \frac{\nu_{max}^2}{\delta} \right)$$

where $\varphi$ is problem-dependent coefficient, $\nu_{max}$ is the maximum value of the fluid velocity, $L_o$ is a characteristic length, $\varphi$ is a body force, and $\delta$ is the relative incompressibility or the density variation factor, which is defined as $\delta = \Delta \rho / \rho_o = \frac{\nu_{max}^2}{c_i^2} = \frac{\nu_{max}^2}{L_o}$, where $M$ is the Mach number. Upon selecting the sound speed much larger than the fluid velocity (at least an order of magnitude) thereby resulting in a very small Mach number, the density variation can be limited to 1% ($\delta \approx 0.01$), which is used in this work. Our own experience as well as other works [35,36] in the literature have indicated that the rules of thumb given by Eq. (17) may not be adequate for some problems. In this case, the problem-dependent coefficient can be used to impose an incompressibility condition for the simulated flow problems. In this presentation, we set $\varphi \approx 4$ where the incompressibility condition is enforced through having density variations less than 1% in the entire computational domain. The speed of sound chosen has a direct effect on the permissible time step in a given simulation.

The algorithm stability is controlled by the Courant–Friedrichs–Lewy (CFL) condition whereby the recommended time step [37] is

$$\Delta t \leq C_{CFL} \frac{h_{\text{min}}}{(c_i + \nu_{max})}$$

where $h_{\text{min}} = 0.5(h_i + h_j)$, $h_{\text{min}}$ is the minimum smoothing length among all $i-j$ particle pairs, and $C_{CFL}$ is a constant satisfying $0 < C_{CFL} \leq 1$ (in this work, $C_{CFL} = 0.125$)

### 4 Problem Description and Boundary Conditions

The modeling domain is composed of a die channel, and an extrudate that are represented by a set of particles as shown in Fig. 1. The length and width of the die channel are $L = 0.2$ m and $H = 0.01$ m, respectively, as indicated in Fig. 2. Initially, the simulation domain is represented by 6600 particles generated by using an array of $200 \times 33$ particles, which is the default number of particles used in all the simulations in this work unless stated otherwise. Henceforth, particles representing solid walls, inlet, outlet, and free surface boundaries are referred to as solid wall boundary particles, die inlet and outlet boundary particles, and free surface boundary particles, respectively. Particles within the die channel as well as the extrudate are called fluid particles. Particles possess all the essential modeling parameters and field variables such as particle position, velocity, density, viscosity, and

![Fig. 1 The simulation domain in particle representation](image)

In order to increment the time-steps in the WCSPH algorithm, we have used a leapfrog predictor corrector method. This technique is an explicit time integration scheme and is relatively simple to implement. Particle positions, densities, and velocities are computed, respectively, as

$$\Delta t \left( \begin{array}{c} \mathbf{r}_i \quad \mathbf{v}_i \quad \rho_i \end{array} \right) = \left( \begin{array}{c} \mathbf{v}_i \\ \mathbf{v}_i \end{array} \right) = \left( \begin{array}{c} \mathbf{v}_i \\ \mathbf{v}_i \end{array} \right)$$

(18)

The time integration scheme starts with the predictor step to compute the intermediate particle positions and densities as follow:

$$\mathbf{r}_i^{(n+1/2)} = \mathbf{r}_i^{(n)} + \frac{\Delta t}{2} \mathbf{v}_i^{(n)}$$

and

$$\rho_i^{(n+1)} = \rho_i^{(n)} + \frac{\Delta t}{2} \rho_i^{(n)}$$

Having computed the intermediate particle positions and densities during the first half time step, the pressure is computed using the previously introduced artificial equation of state, while the velocity is computed by

$$\mathbf{v}_i^{(n+1)} = \frac{\mathbf{v}_i^{(n)} + \mathbf{v}_i^{(n+1)/2}}{2}$$

In the next half time (the corrector step), the particle positions and densities are updated as

$$\mathbf{r}_i^{(n+1)} = \mathbf{r}_i^{(n+1)/2} + \frac{\Delta t}{2} \mathbf{v}_i^{(n+1)}$$

and

$$\rho_i^{(n+1)} = \rho_i^{(n+1)/2} + \frac{\Delta t}{2} \rho_i^{(n+1)}$$

It is to be noted that in the SPH method, the order of particles affects the accuracy of interpolations for gradient and Laplacian computations. Therefore, for computational stability and accuracy, it is preferable to move the particles in a more orderly fashion, which can be achieved through using a velocity variant algorithm also referred to as the XSPH technique suggested by Monaghan [31]. The XSPH method includes the contribution from neighboring particles, thereby enforcing fluid particles to move with an average velocity defined as

$$\mathbf{v}_i^{\text{xsp}} = \mathbf{v}_i - \epsilon \sum_{j=1}^{N} W(\mathbf{r}_{ij}, h) \mathbf{v}_j$$

where $\epsilon$ is a coefficient that varies between 0 and 1. In this study, the coefficient $\epsilon$ is replaced by the average velocity or XSPH velocity $\mathbf{v}_i^{\text{xsp}}$, particle movement only, and $\epsilon = 0.5$. In all times, particles are moved with the $\mathbf{v}_i^{\text{xsp}}$ velocity.

![Fig. 2 The particle distribution on the die channel whose length and width are L = 0.2 m and H = 0.01 m along the x- and y-directions, respectively](image)
pressure. Except solid boundary particles, all particles due to the Lagrangian nature of the SPH approach can move freely in accordance with the solution of the mass and linear momentum balance equations.

The mass and momentum balance equations on the discontinuity surfaces (boundaries) can be formulated, respectively, [38] as 

\[ \| \rho (\vec{V} - \vec{U}) \| \cdot \vec{n} = 0 \text{ and } \| \rho \ddot{V} (\vec{V} - \vec{U}) - \vec{g} \| \cdot \vec{n} = \nabla (\vec{q}) + 2 \Gamma \vec{g} \]  

Here, the symbol \( \| \) indicates the jump of the enclosed quantities across the discontinuity surface; for instance, \( \| \phi \| = \phi^+ - \phi^- \) where \( \phi^+ \) and \( \phi^- \) are the values of \( \phi \) on the positive and negative sides of the discontinuity surface, \( \vec{n} \) is the velocity of the discontinuity surface, \( \vec{n} \) is the unit normal to the discontinuity surface, \( \nabla (\vec{q}) \) is the surface gradient operator, \( \gamma \) is the surface tension, and \( \Gamma \) is the mean curvature. Under the assumptions of no-slip and no-mass penetration boundary conditions for rigid solid walls, the interface mass balance requires that \( v_x = v_y = 0 \). Also assuming no mass penetration across free surfaces as well as ignoring the effect of surface tension, one can reduce the jump condition of the linear momentum balance to \( \| \vec{g} \| \cdot \vec{n} = 0 \) where \( \vec{g} = -p \vec{I} + \vec{T} \). Since the problem in question is the flow of highly viscous fluid into a passive environment with comparatively low viscosity and zero pressure, the free surface boundary condition \( \| \vec{g} \| \cdot \vec{n} = 0 \) is modified to \( \vec{T} \cdot \vec{n} = 0 \), thus implying zero pressure and the stress free boundary condition for the free surface.

The domain boundaries truncate the kernel function of particles that are on or close to the boundaries. Hence, only interior particles will contribute to the SPH approximation for these particles due to the lack of interpolation points on the other side of the boundary. The standard SPH equations introduced in Sec. 3.1, being valid for all interior particles, are partially correct since the kernel function for these particles is no longer a normalized, compact, and spherically symmetric even function. Therefore, the application of boundary conditions correctly and efficiently is quite challenging in the SPH method and necessitates special treatments depending on the type of the boundary. Inaccurate implementation of boundary conditions, for example, results in the penetration of fluid particles into boundary walls and may lead to spurious gradients of field variables, hence, producing errors in the numerical solution since the field variables within the computational domain evolve according to the boundary conditions. In this direction, over the last decade, several different approaches have been suggested to improve boundary treatments that are systematically summarized in various works [19,21,23,33].

Within the context of the SPH method, the solid wall boundaries can be represented by a set of particles. The no-slip boundary conditions on solid boundary walls can be easily implemented by fixing the positions of wall boundary particles and setting their velocities to zero throughout the simulation. In our simulations, we have observed that single layer of wall boundary particles is not sufficient to compute the field variables accurately such as stress, velocity, and pressure; hence, additional layers of solid dummy boundary particles are created parallel to the main wall boundary particles. The overall thickness of these dummy particle layers is set to be at least equal to the radius of the kernel smoothing function. The existence of dummy wall particles helps to reduce the error in computed fields due to the kernel truncation by boundaries. Dummy boundary particles are assigned to zero velocity as well. Both wall boundary and dummy particles behave similarly to fluid particles such that their density and extra stress tensors are computed using the discretization scheme in Eq. (13).

As for the implementation of boundary conditions for the free surface, firstly, the free surface particles should be identified to distinguish them from interior fluid particles. Since the kernel function of particles that are on or in the close vicinity of the free surface is truncated, the particle number density \( n_f \) of these particles will drop. Particles with the number densities below a preset threshold value are recognized as free surface particles: namely,
\( n_i = \sum_{j=1}^{N} W(r_{ij}, h) \) and \( n_{i,\text{ref}} = \max(n_i) \). In SPH modeling, the stress free boundary condition \( \mathbf{T} \cdot \mathbf{n} = 0 \) is automatically satisfied since in evaluating the stress gradient in momentum equation, this term is represented in the residual boundary integration that is cancelled due to the fact that kernel function \( W(r_{ij}, h) \) vanishes beyond its support domain as shown in Eq. (11). Due to the lack of interpolation points or particles outside the free surface, the pressure field computed for the free surface particles can be affected significantly by the spurious pressure gradient. To improve the accuracy of the computed pressure fields, pressure gradients for free surface particles are computed with the assumption of the existence of dummy fluid particles \( j^d \) outside the free surface, which are mirror images of associated interior fluid particles \( j^f \), as shown in Fig. 3.

**Fig. 6** The die swell of Newtonian fluid where color indicates the velocity magnitude.

**Fig. 7** SPH particle distribution for eight possible forms of momentum balance formulations. The results on the left column are obtained by using the Rivlin–Ericksen constitutive equation while those on the right column are obtained by employing the CEF constitutive equation, where (a) covariant convected derivative, (b) contravariant convected derivative, (c) mixed covariant-contravariant convected derivative, and (d) corotational (Jaumann) derivative. Note that in each figure, the particle distributions are colored in accordance with the values of the first normal stress difference \( N_1 \), and the magnitude of the centerline velocity \( v \) is given on each subfigure. The results are obtained using the solution procedure (case 3) expounded below.
In what follows, one can write

\[
\frac{\partial P}{\partial x_i} = \sum_{j=1}^{N} \frac{m_j (P_j' - P_i)}{\rho_j} \frac{\partial W(r_{ij}', h)}{\partial x_i} + \sum_{j=1}^{N} \frac{m_j (P_j' - P_i)}{\rho_j} \frac{\partial W(r_{ij}', h)}{\partial x_i} = 2 \sum_{j=1}^{N} \frac{m_j P_j'}{\rho_j} \frac{\partial W(r_{ij}', h)}{\partial x_i}
\]

where \( \partial W(r_{ij}', h)/\partial x_i = -\partial W(r_{ij}', h)/\partial x_i, P_i = 0, \) and \( P_j' = -P_j', \) which enforce zero pressure boundary condition.

5 Benchmarking Simulations

This section aims at validating the numerical results obtained by the WCSPH method presented. Therefore, we present three benchmark problems, namely Newtonian and non-Newtonian Poiseuille flows and the die swell of a Newtonian fluid. Poiseuille flow consists of two infinitely long stationary plates, parallel to the \( x \)-axis, with a fluid in between them. These plates are separated by a distance \( H, \) where \( y = 0 \) and \( y = H \) are the positions of the bottom and top plates.
respectively. At time $t = 0$, a body force $F_0^B$ is applied to the fluid in the $x$-direction, thereby putting the fluid in motion $v_x(y, t)$. The no-slip boundary conditions are employed at the plate/fluid interfaces $y = 0$ and $y = H$, so that $v_x(0, t) = v_x(H, t) = 0$. The initial condition for all interior particles is taken as $v_x(y, 0) = 0$. For Newtonian incompressible Poiseuille flow, the governing flow equation is the one-dimensional balance of linear momentum equation, $\rho D v_x/Dt = -p_x + \mu (\partial^2 v_x/\partial y^2) + F_0^B$, which can be reduced to $\rho D v_x/Dt = -p_x + \mu \partial^2 v_x/\partial y^2 + F_0^B$ by assuming no variation of $v_x$ in the $x$-direction and noting that $\tau_{xx} = 0$ and $\tau_{xy} = \mu \partial v_x/\partial y$. To initiate the modeling process, a $30 \times 70$ array of particles distributed in $x$- and $y$-directions, respectively, were created in the domain, and the modeling parameters were taken as $H = 10^{-3}$ m, $L = 5 \times 10^{-4}$ m, $F_0^B = 2 \times 10^{-4}$ N/kg, $\rho = 1000$ kg/m$^3$, and $\mu = 10^{-3}$ Pa s. The smoothing length was set equal to 1.6 times the biggest initial particle spacing. The periodic boundary condition is applied for inlet and outlet particles in the direction of the flow. In the WCSPH simulation of a periodic channel flow in literature, the periodic boundary condition is in general imposed such that fluid particles crossing the outlet boundary are reinserted into flow domain at the same $y$-coordinate with the same velocity and density. However, for a relatively long channel, a noticeable pressure loss can be observed along the channel length. In WCSPH, since the pressure field is computed from the density using an artificial equation of state, the outlet boundary pressure poisons the inlet boundary. To circumvent this, the outlet particles are inserted into the flow domain with the same density gradient as at the outlet using the Eq. (20):

$$\rho_l = \left[ \sum_{j=1}^{N} \frac{m_j}{\rho_l} \frac{\partial W(r_{ij}, h)}{\partial x_i} - \left( \frac{\partial \rho_l}{\partial x_i} \right)_{out} \right] \left[ \sum_{j=1}^{N} \frac{m_j}{\rho_l} \frac{\partial W(r_{ij}, h)}{\partial x_i} \right]$$

(20)

An analytical solution to the transient velocity profile for the incompressible Poiseuille flow can be written as [21]

$$v_x(y, t) = \frac{4F_0^B H^2}{\mu \pi} \sum_{k=0}^{\infty} \frac{1}{(2k+1)^2} \sin \left( \frac{(2k+1)\pi y}{H} \right)$$

$$\times \exp \left[ \frac{-(2k+1)^2 \mu \pi^2 t}{2F_0^B} + \frac{F_0^B}{2\mu} (y - H) \right]$$

(21)

which takes on a parabolic velocity profile as $t \to \infty$. Figure 4 illustrates the SPH and analytical transient solutions to the Poiseuille flow problem at various times.

The second test fluid flow problem involves a simulation of one-dimensional, steady state non-Newtonian incompressible Poiseuille flow. As a constitutive equation, we have used Rivlin–Ericksen tensor along with the contravariant form of the convected time derivative. The extra stress tensor of this form can be written in a component form as

$$T_{ij} \tilde{e}_i \tilde{e}_j = \left\{ \mu \left[ v_{ij} + v_{ji} \right] + \frac{D}{Dt} \left[ v_{ij} + v_{ji} \right] - 2v_{im}v_{jm} - v_{im}v_{jm} - v_{im}v_{jm} \right\} \tilde{e}_i \tilde{e}_j$$

(22)

Fig. 9 (a) The magnitude of the velocity versus the axial distance, (b) the magnitude of the velocity as a function of channel width, (c) the shear component $T_{xy}$ of the extra stress tensor, (d) the normal component $T_{xx}$ of the extra stress tensor, (e) the normal component $T_{yy}$ of the extra stress tensor, and (f) the first normal stress difference $N_1$. Results are shown for $x = 0.185$ m.
Equation (22) can be further simplified to the following open forms after using the summation convention and imposing incompressibility condition as:

\[
T_{xx} = 2\mu v_{x,x} + \sigma_1 \left( 2D v_{x,y}/Dt - 4v_{x,y}^2 - 2v_{x,y}^2 - 2v_{x,y}^2 \right) \\
+ \sigma_2 \left( 4v_{x,y}^2 + 2v_{x,y}v_{y,x} + v_{y,y}^2 \right)
\]  
(23)

\[
T_{xy} = \mu (v_{x,y} + v_{y,y}) + \sigma_1 \left( D(v_{y,y} + v_{x,y})/Dt - 2v_{x,y}v_{y,y} - 2v_{x,y}v_{y,y} \right)
\]  
(24)

\[
T_{yy} = 2\mu v_{y,y} + \sigma_1 \left( 2D v_{y,y}/Dt - 4v_{y,y}^2 - 2v_{y,y}^2 - 2v_{y,y}^2 \right) \\
+ \sigma_2 \left( 4v_{y,y}^2 + 2v_{y,y}v_{y,x} + v_{x,y}^2 \right)
\]  
(25)

Casting Eqs. (23), (24), and (25) into the momentum balance in Eq. (1b), the x- and y-components of the balance of linear momentum can be written as.

Fig. 10 Simulation results for the extrudate contraction (left column) and swelling (right column), where (a) the magnitude of the velocity (m/s), (b) the normal component \(T_{xx}\) of the extra stress tensor (Pa), (c) the normal component \(T_{yy}\) of the extra stress tensor (Pa), (d) the shear component \(T_{xy}\) of the extra stress tensor (Pa), and (e) the first normal stress difference \(N_1\) (Pa).
The one-dimensional steady state governing equation can be obtained from Eq. (26) as
\[ \rho \frac{Dv_x}{Dt} = \left\{ \begin{array}{l}
p + \mu \left( v_{x,xx} + v_{y,yy} \right) \\
\frac{D \left( v_{x,xx} + v_{y,yy} \right)}{Dt} - 8v_{y,y}v_{x,yy} - 4v_{x,y}v_{y,yy} - 4v_{x,y}v_{x,yy} \\
-2v_{x,y}v_{y,xx} - 2v_{x,y}v_{x,yy} - 2v_{x,y}v_{y,xy} \\
+ \rho F_x^e \\
\end{array} \right\} + \rho F_x^e \] (26)

The components of the extra stress tensor, \( T_{xx}, T_{yy}, T_{xy} \), can be obtained as
\[ T_{xx} = \frac{\sigma_1}{C_0} \left( v_{x,xx} + v_{y,yy} \right) \]
\[ T_{yy} = \frac{\sigma_1}{C_0} \left( v_{x,xx} + v_{y,yy} \right) \]
\[ T_{xy} = \frac{\sigma_1}{C_0} \left( v_{x,xx} + v_{y,yy} \right) \]

Figure 5 presents the SPH and steady state analytical solutions for the velocity, \( T_{xx} \), and \( T_{yy} \) at the channel length of \( x = 0.1 \) m. The comparison of WCSPH and analytical results shows good agreement, and one, therefore, can conclude that SPH method can capture the flow behavior of a second-order fluid.
To be able to further validate the presented algorithm, the die swell of a Newtonian fluid is also modeled with the subsequent simulation parameters; the channel length and diameter are 0.1 m and 0.01 m, respectively, the density and viscosity of the liquid in the given order are 1000 kg/m$^3$ and 10 Pa·s. The body force is chosen such that the magnitude of the centerline velocity is $7.0 \times 10^{-4}$ m/s, leading to the Reynolds number of $7.0 \times 10^{-4}$, Batchelor et al. [39] experimentally measured die swell of a Newtonian liquid with the Reynolds number of about $10^{-8}$, and reported that the Newtonian liquid has a die swell of 13.5%, which is computed as $100 \times (d_e - d_i)/d_i$ where $d_e$ and $d_i$ channel and the extrudate diameters, respectively. Horsfall [40] attempted to model the experiment in Ref. [38] using a finite difference technique, which produced a die swell of 6.3%. The SPH method predicts the die swell of 6.5% as presented in Fig. 6, which is of very good agreement with the numerical result of Ref. [39], and semiquantitative agreement with the experimental result of Ref. [38]. Due to the computationally expensive nature of the WCSPH method, a single simulation with much smaller Reynolds number ($Re = 10^{-8}$) takes too long. Therefore, for all practical purposes, the SPH die swell simulation is performed at the Reynolds number in the range of $10^{-4}$ with the assumption that there would not be significant differences between results of the die swell at $Re = 10^{-4}$ and $Re = 10^{-8}$.

6 Simulation Results for the Extrudate Swell

This section presents the simulation results of a two-dimensional transient die swell problem under several operating parameters and for various forms of discretization schemes as well as for different formulations of constitutive equations. The model domain and its geometrical parameters have been introduced previously in Sec. 4. The fluid parameters $\rho = 1000\ kg/m^3$, $\mu = 10\ Pa\ s$ are selected for whole simulations. The initial conditions for all interior fluid particles are taken as zero initial velocities. Fluid particles are accelerated from the rest upon the application of a constant body force as described in the benchmark problems. Body force is applied only to fluid particles within the channel. Upon crossing the die channel outlet boundary, fluid particles start moving and deforming freely under the influence of upstream fluid particles. Here, it is worthy of stating that to set the fluid particles in motion, it is also possible to define inlet velocity. Merely due to the convenience and computational simplicity, in this work we have preferred to use body force.

As emphasized in Sec. 2 of the present study, the literature review has shown that there is not a well-established consensus or a guideline regarding the form of a constitutive equation that can be used to model the die swell behavior of the non-Newtonian viscoelastic second-order fluid in extrusion process. In the relevant documented literature [5, 8–10, 25, 26], mainly two different constitutive equations and four different forms of convected derivatives are reported, thereby producing eight possible forms of the momentum balance equation. In the following, we present the findings of a systematic study on the ability of each possible form to predict the die swell phenomenon in an extrusion process. To achieve one to one comparison among all simulation results, the same input parameters are used in each momentum equation. Input parameters are body force $F^\rho_0 = 1881.5\ N/kg$, first and second normal stresses coefficients, $\alpha_1 = -4.0 \times 10^{-3}\ Pa\ m^2$ and, $\alpha_2 = -0.1 \times 10^{-3}\ Pa$. In Fig. 7 is shown the SPH particle distribution both within the die and extrude obtained through the solution of eight possible forms of the momentum balance equations. Colors indicate the values of the first normal stress difference $N_1$ within the channel and the extrude. When results in Fig. 7 are compared against each other, it turns out that the momentum balance equation construction using the Rivlin–Erickson tensor together with the contravariant components of the convected derivative is able to capture the swelling phenomenon satisfactorily, whereas the remaining equations cannot predict a correct trend. Hence, the momentum equation due to “$\alpha_0^\rho\beta_1$” combination was chosen to be a default momentum equation for the benchmark problem already introduced as well as for all other die swell simulations to be presented in coming sections.

In an attempt to find a correct methodology for solving the linear momentum balance equation of a second-order fluid, we have tested four solution procedures that differ from each other in terms of the discretization schemes used and whether the divergence of total stress tensor $\boldsymbol{\sigma}$, extra stress tensor $\mathbf{T}_{ex}$, viscous stress tensor $\tau$ or elastic stress tensor $\varepsilon$ are computed in a single-step (loop) or in two steps. In all two-step methodologies, initially, the components of the velocity gradient are computed using Eq. (13).

- Case 1: having computed the total stress tensor $\boldsymbol{\sigma} = -pI + \tau + \varepsilon$ in the first step, the divergence of the total stress tensor is computed using Eq. (14) in the second step.
- Case 2: after computing the extra stress tensor in the first step, the gradient of the hydrostatic part of the total stress tensor is obtained using Eq. (13), while the divergence of the extra stress tensor $\mathbf{T}_{ex}$ is calculated by using Eq. (14) in the second step.
- Case 3: all three parts of the total stress tensor evaluated individually, where $\nabla \varepsilon$ is evaluated with Eq. (13), $\nabla \tau$ is evaluated as a Laplacian term using Eq. (16) in a single-step, and finally, $\nabla \cdot \varepsilon$ is computed with Eq. (14) in the second step after the computation of elastic part $\varepsilon$ during the first step.

Fig. 12 The results of the extrudate simulation with fine particle numbers for convergence analysis, (a) the shape of the extrudate with colors denoting the velocity magnitude, m/s, and (b) the magnitude of the velocity as a function of channel width, (c) the shear component $T_{xy}$ of the extra stress tensor. Results are shown for $x = 0.185\ m$. 

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Fig. 13 Summary of the die swell simulation with the centerline velocity of 2 m/s, where (a) the magnitude of the velocity (m/s), (b) the normal component $T_{xx}$ of the extra stress tensor (Pa), (c) the normal component $T_{yy}$ of the extra stress tensor (Pa), (d) the shear component $T_{xy}$ of the extra stress tensor (Pa), and (e) the first normal stress difference $N_1$ (Pa).

Fig. 14 (a) The magnitude of the velocity versus the axial distance, (b) the magnitude of the velocity as a function of channel width, (c) the shear component $T_{xy}$ of the extra stress tensor, (d) the normal component $T_{xx}$ of the extra stress tensor, (e) the normal component $T_{yy}$ of the extra stress tensor, and (f) the first normal stress difference $N_1$. Results are shown for $x = 0.185$ m.
• **Case 4**: this is a single-step procedure where each of the first and the second-order derivatives in Eqs. (26) and (27) are individually evaluated using Eqs. (13) and (15).

All four cases have been tested under the same input parameters; namely, the magnitude of the centerline velocity \( v = 3.4 \text{ m/s} \), \( z_1 = -2.8 \times 10^{-3} \text{ Pa.s}^2 \), and \( z_2 = -0.1 \times z_1 \), which produces \( De = 0.0952 \). The results of all relevant simulations led us to conclude that case 1 and case 2 procedures could not predict the correct flow behavior in that fluid particles gradually become unstable especially outside the channel as the simulation progress. On the other hand, case 3 and case 4 result in stable simulations as shown in Figs. 8 and 9.

---

Fig. 15  Particle distributions with colors denoting values of the first normal stress difference \( N_1 \) for Re numbers of 5 and 10, and for various De numbers. The left and right columns for subfigures from (a) to (e) correspond to the centerline velocity of \( v = 5 \text{ m/s} \) and \( v = 10 \text{ m/s} \), respectively. On the other hand, the subfigures (f) and (g) have the centerline velocity of \( v = 10 \text{ m/s} \). Here, (a) \( De = 0 \), (b) \( De = 0.02 \), (c) \( De = 0.1 \), (d) \( De = 0.2 \), (e) \( De = 0.3 \), (f) \( De = 0.4 \), and (g) \( De = 0.5 \).
Simulation results have revealed that the case 4 procedure seems to capture the swelling phenomenon; nevertheless, it is rather sensitive to the magnitude of the De number, and works only for quite small De number values with the upper bound of 0.0952, above which the fluid flow gets highly unstable producing oscillating and perturbed free surface. As well, case 4 does not prove to be the most applicable and effective one in capturing oscillating and perturbed free surface. As well, case 4 does not produce the correct fields. The approach presented in case 3 proves to be the most applicable and effective one in capturing swelling process; hence, it has been used as the default approach for all simulations performed for validations as well as investigating the physics of swell phenomenon. Since the De number used in this set of simulations is rather small, the polymeric fluid did not exhibit noticeable die swell upon being extruded.

The first and the second normal stress coefficients have a significant influence on the behavior of extruded fluid flow. It is important to note that the sign of the first normal stress coefficient \( \sigma_1 \) determines whether the polymeric fluid swells or contracts upon being extruded. For swelling phenomenon to occur, the first normal stress coefficient should be of a negative sign leading to positive \( \sigma_1 > 0 \), while the positive first normal stress coefficient results in negative \( \sigma_1 < 0 \), hence, forcing the polymeric fluid to contract. To be able to test if the developed algorithm can also predict the contraction behavior, we have performed comparative numerical simulation studies with the following input parameters; for simulating swelling process, \( \sigma_1 = -4.0 \times 10^{-3} \text{ Pa} \), \( \sigma_2 = 0.1 \times \sigma_1 \), and \( F_B^a = 1881.5 \text{ N/kg} \), while for the contraction phenomenon, \( \sigma_1 = 4.0 \times 10^{-3} \text{ Pa} \), \( \sigma_2 = 0.1 \times \sigma_1 \), and \( F_B^a = 20,000 \text{ N/kg} \). These parameters produce a centerline velocity of \( v \geq 10.0 \text{ m/s} \), resulting in \( De = 0.4 \).

Figures 10 and 11 present the simulation results for both swelling and contraction cases. When a polymeric fluid is sheared between the walls of the die, it develops tensile stresses along the flow direction (positive \( T_{xx} \)) bringing about positive first normal stress difference \( \sigma_1 > 0 \). This additional stress in the fluid exerts a net force on the walls of the channel. Once the polymeric fluid is extruded through the die, it cannot support this additional stress; hence, the fluid tends to expand in the radial direction. On the other hand, some polymeric fluids when sheared may develop compression along the streamlines (negative \( T_{xx} \)), thereby resulting in negative \( \sigma_1 < 0 \). Hence, normal stresses are responsible for the occurrence of polymer swelling and contraction. An interesting observation to note is that to achieve the same centerline velocity, the body force applied in the simulation of the contraction phenomenon is higher than that used in the swelling case. This is due to the fact that since the fluid element is compressed along the stream line direction (negative \( T_{xx} \)), the body force applied is used for overcoming this compression and keeping the flow in motion.

To show convergence, the extrudate swell test case presented in the right column of Fig. 10 was also repeated using twice as many particles (i.e., 280 × 47 = 13,160) for which results are presented in Fig. 12. Results for both particle resolutions are compared in terms of swelling ratios, the shape of the free surface, and transversal velocity and shear stress distributions within the channel. The comparison of results on the medium and the fine particle numbers demonstrates evidently that the medium particle number provides comparable swelling ratios (i.e., swelling ratios are 1.55 and 1.5 for the medium and fine particle numbers, respectively), and solutions with sufficient accuracy considering the trade-off between computational costs and capturing the features being studied.

To study the effect of velocity on the extrudate swelling, we performed a numerical experiment with the same viscometric parameters, \( \sigma_1 = -4.0 \times 10^{-3} \text{ Pa} \), \( \sigma_2 = 0.1 \times \sigma_1 \) as the die swell test case presented in the right column of Fig. 10. The fluid is accelerated with the body force of \( F_B^a = 1100 \text{ N/kg} \) for the first experiment. The computed centerline velocity magnitude and Deborah number are \( v \approx 2 \text{ m/s} \) and \( De = 0.08 \). It is obvious from the comparison of Fig. 13 with the die swell case given in Fig. 10, and also from Fig. 14 that the rise in the extrusion velocity increases swelling ratio since the first normal stress difference is a function of the shear rate and as the shear rate increases so does the normal stress difference.

**Table 2 Input parameters for simulations with various De and Re numbers**

<table>
<thead>
<tr>
<th>De = ( \frac{\nu}{\mu} )</th>
<th>( \nu \geq 5 \text{ m/s}, \text{ Re} = 5 )</th>
<th>( \nu \geq 10 \text{ m/s}, \text{ Re} = 10 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( F_B^a ) (N/kg)</td>
<td>( \sigma_1 ) (Pa s²)</td>
<td>( F_B^a ) (N/kg)</td>
</tr>
<tr>
<td>0.02</td>
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</tr>
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<td>0.1</td>
<td>3870.0</td>
<td>(-4.0 \times 10^{-4})</td>
</tr>
<tr>
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<td>(-2.0 \times 10^{-3})</td>
</tr>
<tr>
<td>0.3</td>
<td>1710.0</td>
<td>(-4.0 \times 10^{-3})</td>
</tr>
<tr>
<td>0.4</td>
<td>1245.0</td>
<td>(-6.0 \times 10^{-3})</td>
</tr>
<tr>
<td>0.5</td>
<td>815.0</td>
<td>(-4.0 \times 10^{-3})</td>
</tr>
<tr>
<td>0.6</td>
<td>815.0</td>
<td>(-5.0 \times 10^{-3})</td>
</tr>
</tbody>
</table>

**Fig. 16** The swelling ratios at different axial positions \( x = 0.21, 0.23, \) and \( 0.25 \text{ m} \) for different centerline velocities, (a) \( v \geq 5 \text{ m/s} \), (b) \( v \geq 10 \text{ m/s} \), respectively, (c) averaged swelling ratio for \( v \geq 5 \text{ m/s} \) and \( 10 \text{ m/s} \).
In order for examining the effect of Deborah number as well as the inertial effect on the swelling mechanism, we performed two sets of simulations in which two different Reynolds number \( (Re = \frac{\rho V}{\mu}) \) where the characteristic length \( l \) is taken to be channel height \( \) values \( (Re = 5 \text{ and } 10) \) and various \( De \) numbers ranging from 0 to 0.5 are used (see Fig. 15). Simulations parameters employed in the present study are listed in Table 2. Figure 16 summarizes the results of the simulations in terms of the swelling ratio versus Deborah number and clearly shows that the radius of the extrudate jet increases monotonically as the value of \( De \) increases. Results in Fig. 17 suggest that as the normal component of the extra stress tensor increases so does the first normal stress difference, hence, leading to an increase in the diameter of the extrudate in radial direction. Another interesting conclusion that can also be extracted from the given results is that as the \( De \) number increases, the extrudate swell starts at the die exit, while for smaller \( De \) numbers, it is delayed. We have also observed that the inertial force has a significant effect on the swelling diameter. Figure 15 also shows that the swelling obtained from simulations with the centerline velocity of \( \approx 10 \text{ m/s} \) (corresponding to the Re

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![Graphs showing various components of stress](image)

**Fig. 17** The left and right columns, respectively, correspond to the centerline velocities of 5 and 10 m/s, where (a) the shear component \( \tau_{xy} \) of the extra stress tensor, (b) the normal component \( \tau_{xx} \) of the extra stress tensor, (c) the normal component \( \tau_{yy} \) of the extra stress tensor, and (d) the first normal stress difference \( N_1 \). Results are shown for \( x = 0.185 \) m.
It is noted that the WCSPH algorithm presented here has an upper bound for achievable De number. For Reynolds number of 5 and 10, the upper bounds are 0.3, and 0.5, respectively. In simulations with De number values greater than these upper bounds, fluids particles accumulate at the die exit. As the simulation progresses, local fractures in particle distribution start forming at the channel exit, thereby terminating the simulation. It is experimentally well known that as the Deborah number increases, the polymeric fluids start acting more solidlike, thereby experiencing difficulties in its flow nature. As a result, it may experience fracture, which is widely referred to as “melt fracture” in the polymer processing industry. Nevertheless, it is believed that the upper bounds mentioned are not high enough to induce such a physical insight. Therefore, we conclude that these thresholds in obtainable Deborah numbers are of numerical nature. Investigating why WCSPH approach has a threshold in achievable Deborah number is a subject of the future research in this area.

Fig. 18 The summary of the WCSPH simulation for $We_{\text{effective}} = 0.1$ in terms of (a) the velocity magnitude, (b) the first normal stress difference, and (c) the shear component of the extra stress tensor stress. Graphical results are given for $x = 0.180$ m.

Even though the objective of this work is to model the swelling behavior of a second-order fluid when extruded through a channel, for the sake of completeness, we have also tested our algorithm on an Oldroyd-B fluid, and compared the swelling ratio with the one reported in the literature [41]. For this simulation, following input parameters are utilized; the channel diameter and lengths are 0.02 m and 0.2 m, respectively, $\rho = 1000$ kg/m$^3$, $\mu = 10$ Pa s, $\lambda_1 = 0.01$ s, and $\lambda_2 = 0.9 \times \lambda_1$. In this simulation, the initial computational domain is represented by 6200 particles, which are created through an array of 200 x 31 particles in x- and y-directions, respectively. The body force is chosen such that it gives a centerline velocity of $1$ m/s. These input parameters correspond to the Reynolds number $Re = \rho lv / \mu$ and Weissenberg number $We = \frac{l}{\lambda_1}$ of one, and the effective Weissenberg number, $We_{\text{effective}} = (1 - (\lambda_2 / \lambda_1))We$ of 0.1 through using the characteristic length $l$ to be equal to the die radius. Under this simulation conditions, the value of the die swell was reported to be 1.37 in [41], while the WCSPH method predicts the die swell of 1.30. Figure 18 shows the summary of the WCSPH simulation in terms of the velocity magnitude, the first normal stress difference, and the shear component of the extra stress tensor stress.

Concluding Remarks

The SPH method has proven itself to be an effective technique to model second-order and Oldroyd-B fluids with free surface flows as it allows the relatively easy implementation of free surface tracking, which is otherwise difficult in mesh-dependent techniques, and is able to predict swelling behavior of polymeric fluids when extruded through a die. Thus, the SPH method can be considered as a viable and efficient alternative for modeling the extrude swell. It is noted that the field variables and material functions predicted using Rivlin–Ericksen constitutive equation together with the contravariant components of the convected derivative of the viscous stress tensor give rise to a correct trend in swelling behavior of the second-order polymeric fluids. In addition, it was found that the elastic stress tensor should be treated separately and computed in two steps in order to obtain correct results. The effects of various rheological and processing parameters on the swelling phenomenon has been presented such as the magnitude and sign of the first and second normal stress coefficients, velocity of flow, and Deborah number. In light of the simulation results, one can rightfully conclude that the SPH method is able to capture both swelling and contraction behavior of polymeric fluids correctly.

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References


