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Three-dimensional Finite Element Solution of the Flow in Single and Twin-Screw Extruders

This work is aimed at the numerical modeling of the flow inside single and twin-screw extruders. Numerical solutions are obtained using a recently developed immersed boundary finite element method capable of solving the flow in the presence of complex non-stationary solid boundaries. The method is first validated against the solution obtained on a body-conforming grid for a single screw extruder and then applied to a twin-screw mixer. The time dependent single screw problem can also be solved in a rotating reference frame for which a steady state solution can be obtained. This allows the evaluation of time integration errors of the moving immersed interface algorithm. For instance the flow is considered isothermal and the material behaves as a Generalized Newtonian fluid. Because the viscosity depends on the shear rate, solutions will be shown for various rotation velocities of the screw and compared with solutions obtained on body-conforming grids. The method is shown to give very accurate results and can be used for a more in-depth investigation of the material behavior in extruders.

1 Introduction

In injection molding and extrusion, polymers are plasticized (melted by viscous generated heating) inside screw mixers and then pushed into the cavity to form the desired part. Important efforts have been devoted during the last decade to the numerical modeling of the injection molding process with more and more emphasis being given to three-dimensional modeling (Kim and Turg, 2004; Ilinca and Héту, 2001, 2003). Solution of the flow inside the plasticization unit is more difficult because the geometry changes continuously as the screws rotate. A survey of various attempts to solve a 2D analogy of the flow inside twin screw extruders is presented by Kajiwara et al. (1996) and Bravo et al. (2000). An effort in modeling the 2D flow in a single C-shaped chamber of a counter-rotating twin screw extruder is reported by Speur et al. (1987). Kajiwara et al. (1996) developed a 3D numerical technique to simulate fluid flow in the case of full flight conveying screw elements. Their simulations were however restricted to one section of the analysis domain, located in the nip region, and relied upon

periodic boundary conditions. Cheng and Manas-Zloczower (1997, 1998) and Yao and Manas-Zloczower (1998) reported 3D numerical studies of co-rotating twin screw extruders using the commercial software FIDAP. Their approach was based on selecting a number of sequential geometries representing various positions of the screws in order to represent a complete cycle and then computing steady state solutions for each of them. The dispersive mixing efficiency of the flow field was assessed in terms of its elongational flow components and magnitude of shear stresses. Zhang et al. (2009) uses a mesh superposition technique to solve intermeshing twin-screw extruders without remeshing. The procedure, incorporated into the Polyflow software, generates finite element meshes for the flow domain and each screw element, respectively, which are then superimposed. The position of each screw is then updated at each time step. In their study, particle tracking is used to generate the distribution of the residence time inside kneading disks elements. The mixing performance and efficiency is also determined using the framework developed by Ottino et al. (1981). Three-dimensional solutions of the steady state flow and energy equations inside twin-screw extruders are reported by Ishikawa et al. (2000). The Stokes equations describing the polymer flow are solved separately for each flow domain corresponding to successive positions of the screw. The same approach is applied to the energy equation by including the convective term but neglecting the transient effects. One drawback of such an approach is that while the polymer melt may reach a quasi-steady state (or periodic variation), the heat transfer should take into account the coupling between the convective transport and the actual change in the flow domain. Therefore, the steady state solution of the energy equation should only be seen as an approximation of the global heat balance inside the screw extruder. Kalyon and Malik (2005, 2007) used the same steady-state framework to describe the flow and heat transfer of generalized Newtonian fluids inside co-rotating and counter-rotating twin screw extruders. Their studies investigate the pressure distribution inside combinations of multiple screw elements and inside screw-die configurations. Bertrand et al. (2003) presented a fictitious domain method based on a mesh refinement technique overlapping a single reference mesh. The mesh is locally adapted to enrich the discretization in small gaps and applications are shown for 2D flow simulation in twin-screw extruders.

The main hurdle when modeling the flow inside twin-screw extruders is the permanent change in the computational domain determined by the rotation of the screws. Various techniques

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can be used to deal with the time dependent flow domain: global remeshing, addition/deletion of elements based on a reference mesh, fictitious domain or immersed boundary methods. Remeshing and mesh adaptation techniques are used generally in conjunction with solution algorithms based on body-conforming grids. While most industrial solvers use body conforming meshes, there is increasing interest for algorithms using non conforming grids. They are known under the names: immersed boundary, immersed interface, embedded mesh and fictitious domain methods. For simplicity, we will use in the present work the immersed boundary (IB) term to identify a non body-conforming method. These techniques rely on using simple grids on domains of simple shapes with the discretization being performed on a single domain enclosing both fluid and solid regions. It is understood that solid surfaces will intersect the mesh between grid points and that they will not be formally represented by the grid (i.e. by no-slip surfaces at the fluid-solid interface). These methods trade the geometrical complexity of the domain of interest for the simplicity of easy to create geometries using relatively uniform meshes. This necessitates abandoning a simple implementation of boundary conditions for a more complex one.

The IB method was initially introduced by Peskin (1972) which used source terms distributed through the solid region to indirectly enforce the proper boundary conditions on the solid-fluid interface. IB methods received particular attention in recent years. Their applications cover a broad spectrum of fluid dynamics problems from flow through heart devices (Peskin, 1972, 1977) to the interaction of body movement and fluid flow (Mittal and Iaccarino, 2005). Reviews of IB methods can be found in (Mittal and Iaccarino, 2005) and (Margnat and Morinière, 2009). Most of these developments were made using a finite difference framework. IB methods using finite elements were developed more recently (Glowinski et al., 1994) and an overview can be found in (Ilinca and Héty, 2010a). In most IB methods, boundary conditions on immersed surfaces are handled either accurately by using dynamic data structures to add/remove grid points as needed or in an approximate way by imposing the boundary conditions to the grid point closest to the surface or through least-squares. Our recently proposed approach (Ilinca and Héty, 2010a) achieves the level of accuracy of cut cell dynamic node addition techniques with none of their drawbacks (increased CPU time and costly dynamic data structures). This approach was extended to moving fluid/solid interfaces in (Ilinca and Héty, 2010b).

In this work, the isothermal flow inside single- and twin-screw extruders is solved using the 3D finite element IB method developed in (Ilinca and Héty, 2010a, 2010b). The solution is interpolated using linear elements and time integration is done by an implicit Euler scheme. The immersed boundary is represented using a time dependent level-set function using the same linear interpolation functions that are used to solve the flow problem. For low Reynolds number, isothermal, viscous flows, the solution does not depend upon time and the proposed approach can be verified against solutions on body-conforming grids. For high velocity flows, in which convection transport is important, the proposed IB method is shown to predict adequately the flow structures produced by the continuous repositioning of the screw surfaces. Hence, a rigorous framework is established for solving transport phenomena as those

encountered for heat transfer, particle tracking and residence time computations.

The paper is organized as follows. First the model problem and the associated finite element formulation is presented. The IB formulation and the procedure to impose the boundary conditions on moving solid surfaces are discussed briefly in section 3. Section 4 illustrates the performance of the present IB method for the 3-D flow inside screw extruders. The paper ends with conclusions.

2 Model Equations

2.1 Flow Equations

The flow of viscous incompressible fluids is described by the Navier-Stokes equations

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) = -\nabla p + \nabla \cdot [\eta (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] + \mathbf{f}, \quad (1)$$

$$-\nabla \cdot \mathbf{u} = 0, \quad (2)$$

where ρ is the fluid density, t denotes time, $\mathbf{u}$ is the velocity, p is the pressure, η is the dynamic viscosity and $\mathbf{f}$ is a volumetric force vector.

The interface between the fluid and solid regions is defined using a level-set function ψ which is defined as a signed distance function from the immersed interface:

$$\psi(\mathbf{x}) = \begin{cases} d(\mathbf{x}, \mathbf{x}_i), & \mathbf{x} \text{ in the fluid region,} \\ 0, & \mathbf{x} \text{ on the fluid/solid interface,} \\ -d(\mathbf{x}, \mathbf{x}_i), & \mathbf{x} \text{ in the solid region,} \end{cases} \quad (3)$$

where $d(\mathbf{x}, \mathbf{x}_i)$ is the distance between the point $P(\mathbf{x})$ and the fluid/solid interface. Hence, points in the fluid region will take on positive values of ψ , whereas ψ for points in the solid region will be negative.

2.2 Boundary Conditions

The boundary conditions associated to the momentum-continuity equations are

$$\mathbf{u} = \mathbf{U}_d(\mathbf{x}), \quad \text{for } \mathbf{x} \in \Gamma_D, \quad (4)$$

$$\eta (\nabla \mathbf{u} + \nabla \mathbf{u}^T) \cdot \hat{\mathbf{n}} - p \hat{\mathbf{n}} = \mathbf{t}(\mathbf{x}), \quad \text{for } \mathbf{x} \in \Gamma_t, \quad (5)$$

where Γ_D is the portion of the fluid boundary where Dirichlet conditions are imposed, and $\mathbf{t}$ is the traction imposed on the remaining fluid boundary. Dirichlet boundary conditions are also imposed at the interface between fluid and solid regions. Because this interface is not represented by the finite element discretization, a special procedure is used to enforce velocity boundary conditions on this surface. This approach will be discussed in the section 3.

2.3 The Finite Element Formulation

In this work we discretize the momentum-continuity equations using a GLS (Galerkin Least-Squares) method with linear con-

tinuous shape functions for both velocity and pressure. This leads to the following weak formulation: (see Eqs. 6 and 7 at bottom of page) where $\mathbf{v}$ and q are continuous, piecewise linear test functions associated to the velocity and pressure equations. The stabilization parameter τ is computed as from (Tezduyar et al., 1990):

$$\tau = \left[\left(\frac{2\rho|\mathbf{u}|}{h_K} \right)^2 + \left(\frac{4\eta}{m_K h_K^2} \right)^2 \right]^{-1/2}, \quad (8)$$

here h_K is the size of the element K and m_K is a coefficient set to 1/3 for linear elements (Tezduyar et al., 1990; Franca et al., 1992). The GLS method contains additional stabilization terms which are integrated only on the element interiors. These terms provide smooth solutions to convection dominated flows and deal with the velocity-pressure coupling so that equal-order interpolation results in a stable numerical scheme (Hughes et al., 1986; Franca et al., 1992). This makes it possible to use elements that do not satisfy the Babuška–Brezzi condition as is the case of the linear P1–P1 element (Hughes et al., 1986; Tezduyar et al., 1990). GLS also stabilizes the resulting linear systems, making them tractable by robust iterative solvers. This last advantage is very important for large scale applications.

3 The Immersed Boundary Method

In the proposed approach, the computational domain contains the complete volume covered by the system, including moving mechanical parts that are considered a solid region. The mesh is intersected by the fluid/solid interface at points located along element edges and we consider those points as additional degrees of freedom in the finite element formulation. A special treatment is then applied to solid region and interface degrees of freedom. In Fig. 1 the mesh is shown by the continuous lines, the interface is indicated by the discontinuous line and the additional interface nodes are indicated by the square symbols. The technique was implemented for 3-D meshes but for the ease of the presentation only a 2-D case is shown in Fig. 1.

The fluid/solid interface is defined by the level-set function and therefore the additional interface nodes are easily determined as being those for which $\psi = 0$. Moreover, because the level-set function is interpolated using linear shape functions, the intersection between the interface and a tetrahedral element is a plane, either a triangle or a quadrilateral. Elements cut by the interface are therefore decomposed into sub-elements which are either entirely in the fluid or entirely in the solid re-

Fig. 1. Decomposition of interface elements for IB method

gion. The additional degrees of freedom associated to the nodes on the interface would normally determine a modification of the global matrix resulting from the finite element equations. In such a case, the implementation is more challenging and would result in an increase in computational cost inherent to dynamic data structures and renumbering. The present approach does not need the explicit addition of the degrees of freedom associated to those nodes. The degrees of freedom associated to the interface nodes are eliminated at the element level by using the Dirichlet boundary conditions for the velocity and by static condensation for the pressure. Hence, the pressure interpolation is taken continuous except for the element faces cut by the interface where it is discontinuous. The procedure results in the local enrichment of the pressure discretization. For more details regarding the implementation of the IB method the reader may consult (Ilinca and Hétu, 2010a, 2010b).

4 Numerical Applications

In this section the IB solution algorithm is used to solve the flow inside screw extruders. Two distinct flow regimes are investigated. For Stokes flow typical of polymer melts, characterized by negligible inertia compared to viscous forces, the solution does not depend upon time (i.e., for each position of the screws the flow is described by steady state equations). Therefore, such analysis can also be conducted on body-con-

$$\int_{\Omega} \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) \mathbf{v} d\Omega + \int_{\Omega} \eta (\nabla \mathbf{u} + \nabla \mathbf{u}^T) : \nabla \mathbf{v} d\Omega - \int_{\Omega} p \nabla \cdot \mathbf{v} d\Omega - \int_{\Omega} \mathbf{f} \mathbf{v} d\Omega + \sum_K \int_{\Omega_K} \left\{ \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) + \nabla p - \nabla \cdot [\eta (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] - \mathbf{f} \right\} \tau \rho \mathbf{u} \cdot \nabla \mathbf{v} d\Omega_K = \int_{\Gamma_i} \mathbf{t} \cdot \mathbf{v} d\Gamma, \quad (6)$$

$$\int_{\Omega} \nabla \cdot \mathbf{u} q d\Omega + \sum_K \int_{\Omega_K} \left\{ \rho \left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right) + \nabla p - \nabla \cdot [\eta (\nabla \mathbf{u} + \nabla \mathbf{u}^T)] - \mathbf{f} \right\} \tau \nabla q d\Omega_K = 0. \quad (7)$$

forming grids and the accuracy of the IB method can be assessed against that of a standard finite element method. For convective flow problems (Reynolds number $Re > 1$) the solution is time dependent and the IB algorithm should consider the continuous change in the screw position. For the single screw case, a steady state solution can be obtained if one chooses a rotating frame of reference. By comparing the transient rotating screw solutions to the reference one we can evaluate the accuracy of the IB method for time dependent problems. However, the rotating reference frame approach cannot be applied to twin screws and only the IB method will be used in this case.

4.1 Steady State Flow inside a Single Screw Mixer

This problem is inspired from extrusion and injection molding applications in which plastic pellets are mixed in a screw plasticizing unit prior to being injected into a mold. The flow is solved around a single screw rotating at a constant angular speed ω inside a fixed barrel of radius R . The screw profile, illustrated in Fig. 2, has an inner radius $R_i = 0.6R$, outer radius $R_o = 0.98R$ and pitch $L = R$. The profile has a trapezoidal shape with round corners of radius $R_s = 0.05R$.

The level-set function is determined analytically as the signed distance function to the screw surface. The screw surface is given by

$$(y^2 + z^2)^{1/2} = r_{\text{screw}}(x'), \quad (9)$$

where r_{screw} defines the screw profile in the (x, r) plane as shown in Fig. 2 and x' provides the mapping of the screw profile into the 3D, time dependent screw surface position:

$$x' = x + x_0 + x_t, \quad x_0 = L \left(1 - \frac{\theta}{2\pi} \right), \quad x_t = \frac{L\omega t}{2\pi}. \quad (10)$$

The angle $\theta \in [0; 2\pi]$ is the angle made by the vector $y\hat{j} + z\hat{k}$ with the y axis.

A non-dimensional solution is obtained by defining reference values for the variables describing the geometry and the flow. The reference length L_0 is taken equal to the barrel radius R and the reference velocity is given by $U_0 = \omega R$. The advection forces are considered very small when compared to the viscous forces and therefore are neglected. Equations corre-

sponding to the Stokes flow are therefore solved in the following dimensionless form

$$0 = -\tilde{\nabla} \tilde{p} + \tilde{\nabla} \cdot [\tilde{\eta}(\tilde{\nabla} \tilde{\mathbf{u}} + \tilde{\nabla} \tilde{\mathbf{u}}^T)], \quad (11)$$

$$-\tilde{\nabla} \cdot \tilde{\mathbf{u}} = 0, \quad (12)$$

where the dimensionless variables are defined as:

$$\tilde{\nabla} = \frac{\partial}{\partial \tilde{x}} \mathbf{i} + \frac{\partial}{\partial \tilde{y}} \mathbf{j} + \frac{\partial}{\partial \tilde{z}} \mathbf{k}, \quad \tilde{x} = \frac{x}{L_0}, \quad \tilde{y} = \frac{y}{L_0}, \quad \tilde{z} = \frac{z}{L_0},$$

$$\tilde{\mathbf{u}} = \frac{\mathbf{u}}{U_0},$$

$$\tilde{\eta} = \frac{\eta}{\eta_0}, \quad \eta_0 = \eta(\gamma_0), \quad \gamma_0 = \frac{U_0}{L_0},$$

$$\tilde{p} = \frac{p}{p_0}, \quad p_0 = \frac{\eta_0 U_0}{L_0}.$$

The material is considered as behaving as a generalized Newtonian fluid with the viscosity described by the Cross model:

$$\eta(\dot{\gamma}) = \frac{\eta_r}{1 + \left(\frac{\eta_r \dot{\gamma}}{\tau^*} \right)^{1-n}}, \quad (13)$$

where model constants take on values corresponding to polystyrene at 200 °C (Ilinca and Héty, 2001): $n = 0.26$, $\tau^* = 2.5 \cdot 10^4$ Pa, $\eta_r = 3.841 \cdot 10^3$ Pa · s.

Numerical simulations were carried out considering a total screw length $L_s = 4L$. The computational domain spans from $x = 0$ to $x = 4L$ and from $r = 0.5R$ to $r = R$, where $r = (y^2 + z^2)^{1/2}$. Fig. 3 shows the computational domain, with the fluid region shown in transparent gray. A cross-section of the grid at $x = 2L$ is shown in Fig. 3B with the solid region of the grid plotted with lighter gray scale. The mesh has a total of 344 544 nodes and 1 658 880 tetrahedral elements.

The screw is considered as turning anti-clockwise with respect to the section shown in Fig. 3B, thus pushing the material in the negative direction of the x -axis. Screw rotation will therefore generate a pressure build-up towards the left hand side of the screw (negative direction of the x -axis). The screw works under closed discharge, resulting in a zero flow rate across sections normal to the screw axis. Under normal operating conditions the axial flow rate is non-zero, but the axial velocity is one or two orders of magnitude smaller than the screw rotation speed and therefore it was neglected in this study. The following boundary conditions are imposed:

- Non-slip boundary conditions on the barrel surface, $u = v = w = 0$;
- Imposed axial velocity $u = 0$ and zero-traction condition for the v and w velocity components at $x = 4L$. This represents the entry surface and because the screw is under closed discharge conditions, the inlet velocity is zero;
- Zero-traction condition for all velocity components at $x = 0$. This condition will set the zero pressure level on this surface (exit surface);
- Screw velocity $\mathbf{u} = \boldsymbol{\omega} \times \mathbf{r}$ for points inside the screw. Screw rotation speed is $\boldsymbol{\omega} = -\omega \mathbf{i}$, which gives $u = 0$, $v = \omega z$, $w = -\omega y$. The apparent velocity of the screw profile is $\mathbf{u}_a = -L\omega / (2\pi) \mathbf{i}$, which means that the profile is moving in the negative direction of the x -axis by a distance equal to the screw pitch L in a time interval equal to the rotation period $T = 2\pi / \omega$.

Fig. 2. Screw profile for the single screw mixer

Computations were carried out using the IB method and also by a standard finite element method on a body conforming mesh having 337 695 nodes and 1 835 873 elements. Velocity solutions for different rotation speeds are compared in Fig. 4 for the y-component (v) and in Fig. 5 for the z-component (w) in a section at $x = 2L$. In each case the velocity is plotted along the thick black line shown in the left hand side picture, the origin ($y = 0$; $z = 0$) being at the center of the circular barrel section. Results indicate that the agreement with the body-conforming solution is very good for all rotation speeds. Note that the solution depends on the rotation speed due to the shear thinning viscosity of the material.

The pressure distribution on the surface of the screw for $\omega = 100 \text{ s}^{-1}$ is shown in Fig. 6. The dimensionless pressure $\tilde{p} = p/p_0$ is shown. Here again we can observe that the IB solution agrees very well with the solution computed on a body-conforming grid. Because the apparent movement of the screw is towards the left, the pressure is higher on the left side of the screw. The variation along the surface of the barrel at $y = 0$, $z = R$ of the pressure/velocity ratio for various rotation speeds is shown in Fig. 7. The magnitude of the pressure/velocity ratio decreases when the rotation speed increases as a result of a decrease in the viscosity. The dependence of the reference viscosity with the rotation speed is shown in

Fig. 3. Computational domain and screw geometry, (A) 3-D view, (B) cross section at $x = 2L$

Fig. 4. Velocity v profile at $x = 2L$ and $y = 0$ for three different angular velocities

Fig. 5. Velocity w profile at $x = 2L$ and $z = 0$ for three different angular velocities

Fig. 6. Pressure distribution on the screw surface for $\omega = 100 \text{ s}^{-1}$, (A) conforming mesh solution, (B) IB solution

Fig. 7. Pressure along the barrel at $y = 0, z = R$

Fig. 8A, while the variation of the mean pressure gradient along the screw axis is shown in Fig. 8B. At low rotation speed ($\omega < 0.01 \text{ s}^{-1}$) the viscosity is practically constant and the dimensionless pressure gradient changes little with the rotation speed. Because the maximum shear rate is about 50 times higher than the rotation speed, $\gamma_{\max} = \omega R / (R - R_0) = 50\omega$, shear thinning effects are apparent for $\omega > 0.01 \text{ s}^{-1}$. At very high rotation speeds ($\omega > 1000 \text{ s}^{-1}$) the dimensionless pressure gradient changes very little as the material behaves like a power law fluid. However, because in this range of flow conditions the reference pressure decreases with increasing speed as seen in Fig. 8A, the absolute value of the pressure gradient continues to decrease when the screw rotation speed is increased.

Fig. 8. Pressure drop as function of the rotation speed, (A) reference pressure (viscosity), (B) dimensionless pressure gradient

4.2 Transient, Convective Flow inside a Single Screw Mixer

For injection molding and extrusion of polymer melts the material properties and flow regime result in the Reynolds number being smaller than unity, thus making the convective terms in the momentum equations negligible. Such problems can be solved as a succession of steady state conditions (Stokes equations) representing the various positions of the screw. However, transport terms in the energy equation or in equations such as those encountered when solving particle tracking or the solid fraction in powder injection molding cannot be neglected. Also, flow mixing applications involving fluids with much lower viscosity than that of polymer melts may result in a flow regime for which convective terms are important. To verify the general applicability of the proposed approach to flow problems involving moving solid interfaces, the single screw problem was also solved for transient, high velocity conditions for which the convective terms are important. In this case the solution depends with time and simulations were carried out for constant viscosity (Newtonian flow) corresponding to a Reynolds number $Re = \rho U_0 R / \eta = 100$. In the presence of moving interfaces, as in this case, the computational grid remains the same during the course of a simulation but the level set function defining the screw geometry is re-evaluated at each time step. That means ψ is a function of time such as the $\psi(\mathbf{x}, t) = 0$ iso-surface represents the screw surface at time t .

A first computation was carried out using a time step increment $\Delta t = T/40$, with T being the time period of the screw rotation, and then by reducing successively Δt by a factor of two: $\Delta t = T/80, T/160$ and $T/320$. Note that the mesh has 96 elements in circumferential direction, resulting in a CFL number on elements close to the screw surface of 2.4 for the largest

Fig. 9. Velocity component v at $x = 2L$, $y = 0$, (A) v -velocity profile, (B) error with respect to the RRF solution

Fig. 10. Velocity component w at $x = 2L$, $z = 0$, (A) w -velocity profile, (B) error with respect to the RRF solution

time step and of 0.3 for the lowest one. The flow solution was computed for a time interval corresponding to 5 complete screw rotations and it was found that the solution seen from a reference frame rotating with the screw remains practically unchanged after two screw rotations. However, the solution is different when using different values for the time step increment Δt because the fluid/solid interface is relocated continuously as the screw rotates and as the solution changes with time at each grid point.

One way to assess the accuracy of the IB method for various time steps is to compute the flow in a reference frame tied to the screw, for which the geometry does not change with time and therefore having a steady state solution. In this case we use the same IB method and the same grid as for the rotating screw solution, but impose homogeneous Dirichlet conditions for the velocity inside the screw, rotating instead the barrel in the opposite direction, $\omega_b = -\omega$. Hence, the fluid/solid interface remains fixed and the solution converges towards the same steady-state solution for all values of the time step. In the rotating reference frame (RRF) momentum equations should include a source term that takes into account for solving in a non-inertial reference frame. The force $\mathbf{f}$ in Eq. 1 is given by

$$\mathbf{f} = -2\rho\boldsymbol{\omega} \times \mathbf{u} - \rho\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{x}), \quad (14)$$

where $-2\rho\boldsymbol{\omega} \times \mathbf{u}$ is the Coriolis force and $-\rho\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{x})$ is the centrifugal force.

The rotating screw IB solutions for different time step increments are compared with the RRF solution in Fig. 9 and 10. Fig. 9 shows the y -component of the velocity (A) and the error with respect to the RRF solution (B) at $x = 2L$ and $y = 0$. Fig. 10 shows the z -component of the velocity (A) and the error with respect to the RRF solution (B) at $x = 2L$

and $z = 0$. Note that the points ($x = 2L$, $y = 0$, $z = 0.695R$) and ($x = 2L$, $y = 0.6R$, $z = 0$) are on the screw surface. Results indicate that the agreement with the RRF solution is very good and improves when decreasing the time step increment. This can be also seen in Fig. 11 presenting the mean error of the solution for the two cross-sections considered in Fig. 9 and Fig. 10. The slope of the curve $\log(\text{Error}) - \log(\Delta t)$ is very close to the theoretical value of 1 of a first-order Euler implicit scheme. This indicates that the IB method describes accurately the change in the flow domain determined by the rotation of the screw and that the procedure for imposing the boundary conditions on the surface of the screw perform well.

Fig. 11. Mean error of velocity components with respect to RRF solution

4.3 Steady-state Flow inside a Co-rotating Twin-Screw Mixer

In this application, we consider a co-rotating twin screw mixing device in which each screw has the same geometry as the one defined in the previous example. This problem can again be solved on a body-conforming mesh in the case of a Stokes flow because the solution is not affected by the inertial terms. However, as shown for the single screw case,

Fig. 12. Computational domain for the twin-screw mixer

the IB method is general and can be applied to both steady state and transient solutions involving moving fluid/solid interfaces.

The screws are located at a distance $\Delta z = 1.6R$ (measured between their axis of rotation) and the computational domain has a length $L_s = 4L$. Fig. 12 shows the computational domain, with the fluid region shown in transparent gray. A cross-section of the grid at $x = 2L$ is also shown. The mesh has a total of 678 669 nodes and 3 264 000 tetrahedral elements. Both screws rotate in the same direction at angular speed ω . Solutions are computed using the same non-dimensional form of the equations and boundary conditions as for the single screw case.

Fig. 13 shows the y -component of the velocity at $x = 2L$ and $y = 0$, while Fig. 14 shows the z -component of the velocity at $x = L$ and $z = 0$ (see thicker black lines on the left side pictures for the locations where the velocities are plotted). As can be seen, the agreement with the reference solution obtained on a body-conforming grid is very good. Fig. 14 indicates that the flow exchange between the two sides (left and right screws) is high and increases as the rotation speed increases. For rotation speeds $\omega > 1 \text{ s}^{-1}$, the maximum velocity along the vertical line at $x = 2L$ and $z = 0$ is as high as 6 times the reference velocity. Small differences are observed between the IB and body-conforming grid solutions in the region of high velocity, where the velocity gradient is also highest. This may be due to the fact that the IB grid is slightly more refined in this region of the flow.

Fig. 13. Velocity v profile at $x = 2L$ and $y = 0$ (thick black line)

Fig. 14. Velocity w profile at $x = 2L$ and $z = 0$ (thick black line)

Fig. 15. Pressure distribution on the screw surface for $\omega = 100 \text{ s}^{-1}$, (A) conforming mesh solution, (B) IB solution

Fig. 16. Pressure along the barrel

Fig. 17. Pressure drop as function of the rotation speed

The pressure distribution on the surface of the twin-screw extruder for $\omega = 100 \text{ s}^{-1}$ is shown in Fig. 15. Here again we can observe that the IB solution agrees very well with the solution computed on a body-conforming grid. The pressure evolution on the surface of the barrel for $y = 0$, $z = \Delta z/2 + R$ for various rotation speeds is shown in Fig. 16. The magnitude of the dimensionless pressure decreases when the rotation speed increases as a result of a decrease in the viscosity. The variation of the mean pressure gradient along the screw axis is shown in Fig. 17 in dimensionless form. The pressure gradient for the

twin-screw extruder behaves in the same way as was the case for the single screw.

4.4 Transient, Convective Flow inside a Co-rotating Twin-Screw Mixer

This test case is similar to the one described in section 4.2 for the single screw flow. The time dependent solution was computed for constant viscosity corresponding to a Reynolds number $Re = \rho U_0 R / \eta = 100$. A first computation was carried out using a time step increment $\Delta t = T/40$, with T being the time period of the screw rotation, and then by reducing successively Δt by a factor of two: $\Delta t = T/80$, $T/160$, $T/320$ and $T/640$. This problem cannot be solved on a body-conforming grid without extensive remeshing work and therefore the solution for the smallest time step ($T/640$) was used as a reference to which the other solutions are compared.

The position of the two screws at different phases of rotation ($T/4$, $T/2$, $3T/4$ and T) is shown in Fig. 18 for $x = 2L$. The corresponding velocity profile along the horizontal ($y = 0$) and vertical ($z = 0$) sections indicated in Fig. 18 by the thick black lines is presented in Fig. 19. Results correspond to the solution computed with $\Delta t = T/40$. The gap size for the horizontal section (see Fig. 19A) varies between $0.02R$ and $0.4R$. The fluid velocity is given by the screw velocity at the left hand side extremity of the respective section and is zero at the barrel surface ($z = 1.8R$). The vertical section, on the barrel symmetry plane ($z = 0$), spans from $y = -0.6R$ to $y = 0.6R$, at both extremities the velocity being zero (barrel surface). The highest velocity for this section is observed for $t = T/2$ and $t = 3T/2$ when the section is not obstructed by the screws. At $t = T/4$ and $t = 3T/4$ part of this vertical section is occupied by the screws and the flow velocities are smaller.

The IB solutions at $t = (n + 1)T$ (screws position as shown in Fig. 18D) for different time step increments are presented in Fig. 20 and Fig. 21. Fig. 20 shows the y -component of the velocity (A) and the error with respect to the reference solution (B) at $x = 2L$ and $y = 0$. Fig. 21 shows the z -component of the velocity (A) and the error with respect to the reference solution (B) at $x = 2L$ and $z = 0$. The reference solution is the solution with the smallest time step ($\Delta t = T/640$). Results indicate that the solution improves when decreasing the time step increment as expected. This can be also seen in Fig. 22 presenting the mean error of the solution for the two cross-sections considered in Fig. 20 and Fig. 21. The slope of the curve $\log(\text{Error}) - \log(\Delta t)$ is very close to the theoretical value of 1 of a first-order Euler

Fig. 18. Screws position at different times, (A) $t = nT + T/4$, (B) $t = nT + T/2$, (C) $t = nT + 3T/4$, (D) $t = nT + T$

Fig. 19. Velocity profile for various screw position, (A) v -velocity at $y = 0$, (B) w -velocity at $z = 0$

Fig. 20. Velocity component v at $x = 2L$, $y = 0$, (A) v -velocity profile, (B) error with respect to the reference solution

Fig. 21. Velocity component w at $x = 2L$, $z = 0$, (A) w -velocity profile, (B) error with respect to the reference solution

Fig. 22. Mean error of velocity components with respect to the reference solution

implicit scheme. This indicates that the IB method describes accurately the change in the flow domain determined by the rotation of the screws and that the procedure for imposing the boundary conditions on the surface of the screw perform well.

5 Conclusion

An IB finite element method that accurately imposes the boundary conditions on the fluid/solid interface is applied to the solution of single- and twin-screw extruders. The procedure consists of incorporating into the grid the points where the mesh intersects the boundary. The degrees of freedom associated with the additional grid points are then eliminated either because the velocity is known or by static condensation in the case of the pressure.

The three-dimensional IB finite element method was used to solve the flow inside a single-screw mixer and the solution was compared with the one obtained on a body-conforming grid. The IB solution is as accurate as the one computed on a body conforming grid. For a non-Newtonian fluid, the pressure drop along the screw axis depends on the rotation speed. Significant changes were also observed in the velocity distribution when changing the rotation speed. For transient flow at $Re = 100$ the solution improves when the time step decreases.

The flow inside a co-rotating twin-screw extruder is more complex. For a Stokes flow a reference solution can however be computed on a body-conforming grid. The IB method performs again very well and the accuracy is similar to the one observed for the body-conforming grid solution.

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