A coupled finite volume immersed boundary method for simulating 3D viscoelastic flows in complex geometries

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Abstract

We report on simulations of an unsteady three dimensional viscoelastic fluid flow through a model porous medium, employing a finite volume methodology (FVM) with a staggered grid. Boundary conditions at the walls of the porous structures are imposed using a second order immersed boundary method (IBM), allowing for accurate simulations using a relatively coarse grid. We compare the viscoelastic stresses obtained using this new IBM technique with those published in literature and find good correspondence. Next, we applied this methodology to model viscoelastic fluids with a FENE-P constitutive model flowing through closely spaced cylinders. Using periodic boundary conditions, we modeled the flow behavior for Newtonian and viscoelastic fluids for successive contractions and expansions. We observe the presence of counter-rotating vortices in between the closely spaced cylinders. The viscoelastic flow structure is symmetric for lower Deborah (De) number, but onset of an asymmetry occurs after a critical De for an infinite array of cylinders. In the presence of side walls, we observe that the onset of flow asymmetry happens at a much lower De, which can be related to higher viscoelastic stresses normal to the flow direction and larger extensional viscosities which affect the curved streamlines. The three-dimensional flow characteristics for viscoelastic flow at higher De number is quite different in comparison with Newtonian flow behavior.

1. Introduction

Understanding viscoelastic flow is of primary importance for applications such as polymer extrusion, food processing and enhanced oil recovery. It is also of fundamental interest to the scientific community because of the additional complexity as a consequence of the non-Newtonian rheology.

A large amount of experimental studies has been performed to obtain the flow characteristics of viscoelastic fluids in model porous media. These studies used different model geometries, which are mostly contraction-expansion geometries, cavities and slits. Flow past a single sphere, cylinder or an array of cylinders in a two dimensional environment has also been of interest in recent studies [1, 2]. Chmielewski and Jayaraman [3] studied the flow of an elastic liquid through arrays of cylinders with a triangular or rectangular pitch. Their experiments were performed for a porosity of 0.70. Talwar and Khomami [4] experimentally observed the viscoelastic flow behavior around a periodic array of cylinders and found a flow transition from
stable 2D to unstable 3D flow after a critical Deborah number. Microfluidic devices have also found their application in studying the flow dynamics of complex fluids in porous media [5,6].

Because of the severe computational demands, numerical simulations of viscoelastic flows are often limited to two dimensional systems. For example, viscoelastic flow around an infinitely long cylinder (represented by a circle in a two dimensional simulation) has been studied in detail [7, 8]. Alves et al. [8] performed finite volume method (FVM) simulations for flow past a cylinder with a collocated grid arrangement and high resolution schemes (MINMOD and SMART) to represent the convective terms. Oliveira et al. [9] studied two dimensional viscoelastic flow past a bounded single cylinder at very low Reynolds number. A numerical and experimental study of viscoelastic flow past a confined cylinder was conducted by Ribeiro et al. [10] for different aspect ratios of the cylinder. Also finite element methods (FEM) based simulation of viscoelastic flows have been performed for flow around a cylinder [11-13]. Liu et al. [11] used the FEM technique with an elastic viscous split-stress gradient (EVSS-G) methodology to study viscoelastic flow behavior around a linear periodic array of cylinders using FENE type of constitutive equation. Though experimentally [12] for a non-Newtonian flow a higher pressure drop is observed after a certain De number, it is still very difficult to numerically reproduce the results with the present constitutive models [13]. Smith et al. [14] performed a linear stability analysis for a linear array of cylinders. They used a FEM-based algorithm for an Oldroyd-B fluid and reported a transition in flow behavior from steady 2D flow to an unsteady 3D flow after a critical Deborah number. Keunings et al. [15] applied FEM based method to simulate viscoelastic fluid through a contraction geometry. Hulsen et al. [16] implemented log conformational approach on FEM platform to model viscoelastic fluid flow at higher Weissenberg number. Choi et al. [17] applied an extended finite element method to model viscoelastic fluid with suspended particles. A comparison of different FEM based methods to solve viscoelastic fluid problems is shown in the work of Baaijens et al. [18]. Richter et al. [19] numerically studied three dimensional viscoelastic flow past a cylinder but their focus was mostly on hydrodynamics at higher Reynolds number. Sahin et al. [20] performed a two dimensional linear stability analysis of a viscoelastic fluid through an array of cylinders using a semi staggered finite volume based method for different cylinder spacing. Smooth particle hydrodynamics (SPH) methods have been recently applied to study viscoelastic flow in periodic array of cylinders [21]. Yatou [22] studied the flow pattern transition from 2D to 3D flow structures numerically for two dimensional curvilinear viscoelastic flows.

In summary, many simulations have been limited to 2D viscoelastic flows, although three dimensional flow structures for viscoelastic fluids are very different and more unstable compared to its 3D Newtonian fluid counterpart [23-25]. Importantly, in 2D simulations the wall effects in the third direction are (necessarily) neglected. Recently the onset of elastic instabilities for complex flow structures and curved streamlines has been reported [26, 27]. The concept of elastic turbulence in relation with elastic instabilities for polymeric flow has been reported by Groisman et al. [28]. In case of a Taylor – Couette flow for viscoelastic fluids an extra hoop stress is produced due to the radial velocity variations, as shown by Groisman et al. [29].
In this work we report on direct numerical simulations which use a regular Eulerian grid to solve flow of the viscoelastic fluid phase, while coupling with walls and immersed objects is accomplished through a second order accurate immersed boundary method (IBM). The advantage of IBM lies in the fact that no body conforming meshing is needed. Therefore it is easy to implement and the method can be used for rigid as well as moving bodies, even if the geometry is complex. The immersed boundary method has obtained significant attention in the field of Newtonian fluid mechanics (Peskin et al. [30], Mittal et al. [31]), but in the field of non-Newtonian fluid mechanics its application has been limited. The IB method can be efficiently used to model static or moving particles for a fixed structured mesh. Two main classes of IB methods can be found in the literature, namely continuous force methods (CFM) and discrete (or direct) forcing method (DFM). In CFM, as first introduced by Peskin [30], local source terms in the momentum equations are applied. The value of this source term is maximum at the location of the surface of the solid objects and distributed to the vicinity on the immersed boundary by means of a smoothed Dirac delta function. Although the implementation is rather straightforward, the choice of the parameters to tune the fluid-solid interaction is non-trivial (Deen et al., [32]). DFM was first introduced by Mohd-Yusof [33]. In DFM source terms are calculated from the discretized transport equations. Discrete force points are distributed over the surface of an immersed object to maintain the boundary conditions. Uhlmann [34] introduced a combination of both CFM and DFM. In the Uhlmann method a regularized delta function is used to distribute the force density from the Lagrangian force point to the Eulerian mesh. Although this method has been used effectively, the main disadvantage of the method is that the applied force is distributed in a diffusive manner to a volume which is slightly larger than the volume of an actual particle. Hence the calculated particle size is larger and a calibration is needed which may lead to computational inaccuracy. Deen et al. [35] proposed a ghost-cell methodology to prevent the problem of diffuse forcing. In this method the different conserved variables at points inside the particle are calculated by extrapolating the values from the two nodes closest to the particle surface and the boundary value. Hence a second order fully implicit method is formulated. The essential feature of this scheme is that no explicit forcing terms or marker points are added. Rather, no-slip boundary conditions are enforced at the level of the discretized momentum equations of the fluid, by extrapolating the velocity field along each Cartesian direction towards the body surface using a second order polynomial. For viscoelastic fluid modelling one of the most important aspects is a correct fluid-solid coupling. In this paper we describe our extension of the Deen et al. [32] IBM to viscoelastic flow simulation. This IB method used for the fluid solid coupling for the viscoelastic fluid will be discussed in detail in section 2.3.2.

The organization of the paper is as follows. First, we describe our numerical algorithm for viscoelastic fluid flow and our IBM implementation. In the subsequent sections we verify our numerical technique with literature results [8] for a benchmark case study of two dimensional flow past a cylinder. In the final part we show the application of this methodology to a three dimensional Newtonian and viscoelastic flow over a periodic array of cylinders with and without side walls. We will show that the presence of side walls causes the onset of flow asymmetry to occur at much lower Deborah number.
2. Governing Equations

2.1. Constitutive Equations

The fundamental equations for an isothermal incompressible viscoelastic flow consist of a continuity equation, momentum equation and a constitutive equation for the non-Newtonian stress components. The first two are given by:

\[ \nabla \cdot \mathbf{u} = 0 \]  \hspace{1cm} (1)

\[ \rho \left[ \frac{\partial \mathbf{u}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{u} \right] = -\nabla p + 2\eta_v \nabla \cdot \mathbf{D} + \nabla \cdot \mathbf{\tau} \]  \hspace{1cm} (2)

Here \( \mathbf{u} \) is the velocity vector, \( \rho \) is the fluid density (assumed to be constant) and \( p \) is the pressure. \( \mathbf{\tau} \) is the viscoelastic stress tensor. Note that we have explicitly added the Newtonian solvent contribution to the stress as \( 2\eta_s \mathbf{D} \), where \( \mathbf{D} = (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) / 2 \) is the rate of deformation and where the solvent viscosity \( \eta_s \) is assumed to remain constant. The viscoelastic stress must be modeled through a constitutive equation. Here we will use the FENE-P model, which is based on the finitely extensible non–linear elastic dumbbell for polymeric materials, as explained in detail by Bird et al. [36]. Other basic rheological models, such as the Maxwell model and Oldroyd–B model, take the elastic force between the beads to be proportional to the separation between the beads. These types of models have the disadvantage that the dumbbells can be stretched indefinitely, leading to a breakdown in strong extensional flow. To overcome this problem a non-linear spring is implemented to limit the dumbbell extension to a maximum value. The equation derived from molecular theory. The basic form of the FENE-P constitutive equation is:

\[ f(\mathbf{\tau}) \mathbf{\tau} + \lambda \mathbf{\tau} = 2a\eta_p \mathbf{D}, \quad \text{with:} \quad f(\mathbf{\tau}) = 1 + \frac{3a + \left( \lambda / \eta_p \right) \text{tr}(\mathbf{\tau})}{L^2}, \quad a = \frac{L^2}{L^2 - 3} \]  \hspace{1cm} (3)

In equation (3) the operator \( \nabla \) above a tensor represents the convective derivative, defined as

\[ \nabla \mathbf{\tau} = \frac{\partial \mathbf{\tau}}{\partial t} + \mathbf{u} \cdot \nabla \mathbf{\tau} - \nabla \mathbf{u}^T \cdot \mathbf{\tau} - \mathbf{\tau} \cdot \nabla \mathbf{u} \]  \hspace{1cm} (4)

In equation (3) the constant \( \lambda \) is the relaxation time of the polymer, \( \eta_p \) is the zero-shear rate polymer viscosity, \( \text{tr}(\mathbf{\tau}) \) denotes the trace of stress tensor, and \( L \) characterizes the maximum polymer extensibility. This parameter equals the maximum length of a FENE dumbbell made dimensionless by the equilibrium length of a polymer spring. When \( L^2 \to \infty \) the Oldroyd–B model is recovered. The total zero shear rate viscosity is given as \( \eta = \eta_s + \eta_p \). The viscosity ratio, which is actually a measure of polymer concentration is given as \( \beta = \eta_s / \eta \).
2.2. Numerical approach

We will first describe the flow solver and the handling of the viscoelastic stress, followed by a detailed description of our IBM methodology and its implementation.

We simulate a three dimensional (3D) unsteady viscoelastic flow by using computational fluid dynamics (CFD). The primitive variables used in the formulation of the model are velocity, pressure and polymer stress. All the mass and momentum equations are considered and discretized in space and time. A finite volume method (FVM) with a staggered grid is applied. In the FVM, the computational domain is divided into small control volumes $\Delta V$ and the primitive variables are solved in the control volumes in an integral form over a time interval $\Delta t$. The FVM formulation is a well-known methodology to discretize the Navier-Stokes equation, and has been applied before to viscoelastic flow simulations [37].

Figure 1. Location of primitive variables in a 3D fluid cell.

The advantage of using FVM with a staggered grid is that it reduces (checkerboard) pressure oscillations and also is very simple to couple with our second order accurate IBM implementation. The location of all the primitive variables in a 3D cell are indicated in figure 1. The velocity components $u, v, w$ are located at the faces while pressure $p$ and stress $\tau$ variables are located at the center of the cubic cell.

The viscoelastic phase equations are solved in three dimensions (3D) on a Cartesian staggered grid. We apply the discrete elastic viscous stress splitting scheme (DEVSS), originally proposed by Guénette and Fortin [38], to introduce the viscoelastic stress terms in the Navier-Stokes equation because it stabilizes the momentum equation, which is especially important at larger polymer stresses (small $\beta$). A uniform grid spacing is used in all directions. The temporal discretization for the momentum equation is as follows,

$$\rho u^{n+1} = \rho u^n + \Delta t \left\{ -\nabla p^{n+1} - \left[ C_{f}^{n+1} + (C_{m}^n - C_{f}^n) \right] + \left[ (\eta_s + \eta_p) \nabla^2 u^{n+1} + \nabla \cdot \tau^n \right] + \rho g - E^n_p \right\}$$

(5)

Here $\eta_p \nabla^2 u^{n+1}$ and $E^n_p = \eta_p \nabla^2 u^n$ are the extra variables we introduce to obtain numerical stability. $n$ indicates the time index. $C$ represents the net convective momentum flux given by:
\[ C = \rho (\nabla \cdot \mathbf{u}u) \] 

In the calculation of convective term a deferred correction method is implemented. Here the first order upwind scheme is used for the implicit evaluation of the convection term \( (\mathbf{C}_u) \). The deferred correction contribution that is used to achieve second order spatial accuracy while maintaining stability is \( \left( \mathbf{C}_m^n - \mathbf{C}_u^n \right) \) and is treated explicitly. In this expression \( \mathbf{C}_m^n \) indicates the convective term evaluated by the total variation diminishing min-mod scheme. A second order central difference (CD) scheme is used for the discretization of diffusive terms.

In equation (5) the viscoelastic stress part \( \tau \) is calculated by solving equation (3). The viscoelastic stress tensors are all located in the center of a fluid cell, and interpolated appropriately during the velocity updates. The convective part of equation (3) is solved by using the higher order upwind scheme.

Equation (5) is solved by a fractional step method, where the tentative velocity field in the first step is computed from:

\[
\rho \mathbf{u}^{**} = \rho \mathbf{u}^n + \Delta t \left\{ -\nabla p^{n+1} - \left[ \mathbf{C}_f^n + \left( \mathbf{C}_m^n - \mathbf{C}_u^n \right) \right] + \left[ \left( \eta_1 + \eta_2 \right) \nabla^2 \mathbf{u}^{**} + \nabla \cdot \mathbf{\tau}^n \right] + \rho \mathbf{g} - \mathbf{E}_p^n \right\} 
\] 

In equation (7) we need to solve a set of linear equations. The enforcement of a no slip boundary condition at the surface of the immersed boundaries is handled at the level of the discretized momentum equations. This is a crucial part of the method, and is discussed in detail in the following section (2.4). We use a robust and efficient block – incomplete Cholesky conjugate gradient (B-ICCG) algorithm [39-41] to solve the resulting sparse matrix for each velocity component in a parallel computational environment. The velocity at the new time step \( n + 1 \) is related to the tentative velocity is as follows:

\[
\mathbf{u}^{n+1} = \mathbf{u}^{**} - \frac{\Delta t}{\rho} \nabla (\delta p) 
\] 

Where \( \delta p = p^{n+1} - p^n \), is the pressure correction. As \( \mathbf{u}^{n+1} \) should satisfy the equation of continuity, the pressure Poisson equation is calculated as:

\[
\nabla \cdot \left\{ \frac{\Delta t}{\rho} \nabla (\delta p) \right\} = \nabla \cdot \mathbf{u}^{**} 
\] 

This is again solved using the B-ICCG solver. The solver iterations are performed until the norm of the residual matrix is less than the convergence criteria, which is set at \( 10^{-14} \) for our simulations.
As the viscoelastic stress tensor components are coupled amongst themselves and with the momentum equation, the velocity at the new time level \( \mathbf{u}^{n+1} \) is used to calculate the stress value accordingly.

As a steady state criterion, the relative change of velocity and stress components between two subsequent time steps are computed in all the cells in a longer time range. If the magnitude of the relative change is less than \( 10^{-4} \) the simulation is stopped.

2.3. Boundary conditions

2.3.1 External boundary conditions
For the verification case we use an inflow boundary condition at the inlet and a constant pressure boundary at the outlet. No-slip velocity boundary conditions are imposed at solid external walls. No specific stress boundary conditions are implemented at the solid wall.

For the case of flow through a regular array of cylinders, we use periodic boundary conditions. Periodic boundary conditions enable us to mimic an infinitely large model porous medium. We apply a constant body force to impose a flow in the system. We will compare two cases: one with and one without the presence of external side walls.

2.3.2 No-slip boundary conditions for immersed solid objects
No-slip velocity boundary conditions at the interface between the viscoelastic fluid and solid objects are imposed through the immersed boundary method (IBM). The advantage of using IBM is that the use of a body conforming grid is not required. To still ensure a relatively high accuracy, we will use a coupling method which works directly at the level of the discretized momentum equation (5). The discrete representation of the momentum equation is given by

\[
a_c \phi_c + \sum_{nb} a_{nb} \phi_{nb} = b_c
\]

(10)

where \( \phi \) is a fluid phase variable (in this case a component of the fluid velocity). This equation indicates that the value of \( \phi \) for a fluid node “\( c \)” outside of the immersed object can be related to the values of its neighboring nodes “\( nb \)”, some of which may lie inside the immersed object.

In more detail, for a stationary immersed object the implicit \((n+1)\) viscous term in the discretized momentum equation (5) leads to the following coefficients in equation (10):

\[
a_j = \frac{-\Delta t}{2\Delta x_j^2} \Gamma_j
\]

(11)

\[
a_c = 1 - \sum_{nb} a_{nb}
\]

(12)
Here $\Gamma_j$ is the relevant transport coefficient, in this case $(\eta_s + \eta_p) / \rho$. The index $j$ represents the coordinate direction in which the neighboring cell is located. All the other (explicit) terms are contained in the term $h_j$. For a particular fluid node the six surrounding nodes “nb” are first tested to see whether any of these node is a solid node (i.e. lies inside an immersed object). In that case a boundary condition is employed where the value of $\phi_{nb} = \phi_0$ extrapolated to that particular solid node is determined from a linear combination of $\phi$ values of relevant fluid nodes $\phi_1$ and $\phi_2$. Along each Cartesian direction we can introduce a dimensionless coordinate $\xi$ with $\xi = 1$ at the fluid node “c” of interest, $\xi = 0$ at the neighbor node located inside the immersed object, and $\xi = 2$ at the neighboring fluid node. A schematic representation of this coordinate is shown in Figure 2.

![Figure 2. Immerged boundary method implementation strategy for a fluid variable $\phi$.](image)

Next we use a second order interpolation to describe the value of $\phi$ as a function of this coordinate:

$$\phi(\xi) = \frac{1}{2}(1-\xi)(2-\xi)\phi_0 + \xi(2-\xi)\phi_1 + \frac{1}{2}\xi(\xi-1)\phi_2$$

(13)

If $\xi_s$ represents the dimensionless position of the boundary of the solid particle and $\phi_p$ the known boundary value at that point, then the extrapolated value inside the solid, $\phi_0$, can estimated from the second order polynomial as

$$\phi_0 = \frac{2\phi_p - 2\xi_s(2-\xi_s)\phi_1 - \xi_s(\xi_s-1)\phi_2}{(1-\xi_s)(2-\xi_s)}.$$  

(14)

Lastly, $\phi_0$ can be eliminated from equation (10) using equation (14). For a 3-point 1 dimensional stencil, this leads to changed coefficients and a changed right-hand-side as follows:
\[ \hat{a}_2 = a_2 \left( 1 + \frac{\xi}{(2 - \xi)} \right) \]
\[ \hat{a}_1 = a_e - a_0 \frac{2\xi}{(1 - \xi)} \]
\[ \hat{b}_e = \phi - a_0 \frac{2}{(1 - \xi)(2 - \xi)} \phi \]

This method is carried out for all solid nodes to ensure that the boundary condition is properly satisfied for all the solid nodes. The interpolation direction depends on the location of the solid cell neighboring a particular fluid cell. In the current staggered grid implementation, for a fluid u-velocity (x-component of the velocity) in a control volume, if the neighboring solid cell lies at the north, for this particular fluid cell the interpolation direction will be in the +y direction. Similarly for a fluid v-velocity (y-component of the velocity), if the neighboring solid cell is at the west of the fluid cell, the interpolation direction will be in the -x direction. It may also happen for some fluid cell that both north and west are solid neighbors. In that case we have to do interpolation in both +y and -x direction. For moving particles the solid node detection mechanism needs to be performed at each time step. Moreover, note that the above treatment is only well-defined when the surfaces of immersed boundaries are at least two grid cells apart for a 3-point stencil. If there is only a single grid cell in between two surfaces, other rules must be devised (such as less accurate first order interpolation). In this paper we do not encounter either of these complexities because we will consider fixed solid objects with sufficient spacing between the surfaces. For more details on IBM implementation we refer to the paper by Deen et al. [32]

### 2.4. Verification study: Two dimensional flow past a cylinder

To verify the implementation of our method, we perform simulations of viscoelastic flow past a cylinder placed in the center of a straight two-dimensional channel. Boundary conditions between the fluid and cylinder are handled by the immersed boundary method as explained in section (2.3). A schematic representation of the flow geometry is given in figure 3. The distance from the channel inlet to the center of the cylinder \((L_1)\) is \(10R\). The total channel length \((L_2)\) is \(40R\). The height of the channel is \(H=4R\).

![Figure 3. Geometry of channel with a cylinder.](image-url)
We impose a fully developed parabolic velocity profile at the inlet and a constant pressure boundary at the outlet. A no slip boundary condition for velocity is implemented at both side walls of the channel. The two most important dimensionless numbers are the Reynolds number (Re) and Deborah number (De) for our case study. The Reynolds number is the ratio of viscous and inertial forces and kept constant at 0.067 for this case:

\[ \text{Re} = \frac{\rho U R}{\eta} \]

Where \( U \) is the average velocity at the channel inlet and \( R \) is the radius of the cylinder. The De number is the ratio of relaxation time of the polymer (\( \lambda \)) and the characteristic time scale of flow, and is defined as:

\[ \text{De} = \frac{\lambda U}{R} \]

The input parameters of our simulations are kept similar to the work of Alves et al. [8], with minor deviations which we expect will not significantly change the results. In particular, the Reynolds number in our simulation is kept at 0.067 and the viscosity ratio \( \beta \) is set to 0.60, while in the simulations of Alves et al. [8] the Re number was 0 and the viscosity ratio \( \beta \) was set to 0.59. In both cases, at such low Re numbers inertia effects are negligible. The blockage ratio \( R/H \) and channel length are chosen equal to the simulations of Alves et al. [8]. The Deborah number was varied by changing \( \lambda \) and keeping the average inlet velocity constant. We have performed our simulations for three different meshes M1, M2 and M3 with mesh spacings: \( \Delta = R/24 \), \( \Delta = R/36 \) and \( \Delta = R/48 \), respectively, taking care that the CFL criteria are kept around 0.10.

The axial velocity profiles along the centerline behind the cylinder for three different Deborah numbers (De = 0.0 (Newtonian), 0.6 and 0.9) are shown in figure 4 for meshes M2 and M3. We observe only very minor differences in our velocity field for the different mesh spacings. This shows that the results are nearly mesh independent.
The axial velocity profile along the centerline of the channel is plotted in Figure 5 for the Newtonian and Oldroyd-B fluid. As expected for creeping flow, the Newtonian fluid exhibits a symmetrical flow behavior upstream and downstream of the cylinder. For the Oldroyd-B fluid, however, a loss of symmetry takes place in the downstream direction due to the effects of elasticity. Physically, when the polymeric liquid flows past the cylinder the polymer coils get extended. While being stretched, they are also convected into the wake behind the cylinder. In this wake region the polymer coils want to relax back to their equilibrium length. This tendency to contract gives rise to elastic stresses that causes the velocities to be lower than in the situation without elastic stresses. The size of the downstream recovery zone increases with increasing De number except near the rear stagnation point close to the cylinder. Figure 5 also
compares these results with the work of Alves et al. [8]. We find a close agreement for the Newtonian case (De=0) and De numbers 0.6 and 0.9.

Figure 6. Normalized stress profiles behind the cylinder along the channel centerline for different De numbers for an Oldroyd-B fluid

Figure 6 shows the profiles of the longitudinal normal stress component \( \tau_{xx} \) as a function of position along the centerline behind the cylinder for De numbers ranging from 0.1 to 1.0. The maximum stress values increase steadily with higher De numbers due to the fluid elasticity. We compare our stress profiles with Alves et al [8]. Generally the agreement is good. The largest deviation is found at De 1.0, where we observe that our maximum stress prediction is 4% lower compared to the work of Alves et al. [8]. Our maximum stress predictions are also lower compared to the results of Hulsen et al [16], which are the most accurate results to date. In fact, our results are relatively closer to the older results of Alves et al. [8], who also used a locally refined mesh near the cylinder which however was coarser than that of Hulsen et al [16]. So we conclude that the deviation of the predicted maximum is due to a lack of mesh resolution of our uniform mesh. Despite the fact that we use a relatively coarse and uniform mesh overall, these results are very acceptable. This gives us confidence that our method will give valuable results for complicated geometries such as porous structures, where locally refined meshes adapted to the flow structures may be difficult to implement.

3. 3D viscoelastic flow past periodic array of cylinders

3.1. Problem description

We now apply our method to study three-dimensional viscoelastic flow through a highly idealized porous medium represented by a specific arrangement of cylinders. This arrangement forces the viscoelastic fluid to periodically undergo contraction and expansion. In such a flow the extensional behavior of the fluid also becomes very important, apart from its shear behavior.
We study two different cases. The first case uses periodic boundary conditions on all domain boundaries, effectively simulating an infinite array of infinitely long cylinders. The second case uses walls that cut the long axes of the cylinders and periodic boundaries in the other 2 directions, i.e. an infinite array of cylinders confined between two planar walls.

Figure 7. Flow geometry for continuous array of cylinders.

Figure 7 shows the arrangement of cylinders. The radius of a cylinder is defined as $R_c$. The distance in the flow direction ($x$) between two consecutive cylinders $L_c$ is kept at $2.5R_c$. The half-height $H_c$ is kept at $1.5R_c$. The distance between the two side walls $W_c$ is kept at $4R_c$. The flow is driven by a constant body force exerted on the fluid.

We simulate both a Newtonian fluid and a FENE-P viscoelastic fluid, as described in section 2. We use a constant extensional parameter ($L^2$) of 100. The viscosity ratio $\beta$ is kept at 0.02, so the flow has a very strong elastic effect. In all our simulations we kept the Re number at a low value of 0.01, ensuring we are always in the creeping flow regime and any type of inertial effects will be insignificant. We have performed simulations for De numbers ($De = \frac{\dot{\lambda}U}{R_c}$ based on the cylinder radius and mean flow velocity) ranging from 0 to 2.0.

We performed simulations for three different mesh sizes of $\Delta = R_c/24$, $\Delta = R_c/36$ and $\Delta = R_c/48$, respectively. The results for $\Delta = R_c/36$ and $\Delta = R_c/48$ were virtually indistinguishable (not shown). Thus all results in the remainder of this paper are based on the mesh size $\Delta = R_c/36$. It should be noted that we needed to keep the CFL number lower than 0.01 in all our simulations, leading to considerable computational costs. Even at a relatively high De number of 2.0 we did not encounter any stress or velocity divergence. At lower De number a larger time step can be utilized but at De number in range of 1.0 and higher, lower time step is required for better convergence.

We will show that the side walls have a strong influence on the flow structure in such a periodic domain. The presence of side walls actually expedites the process of onset of asymmetry in the flow domain. We will also show that higher elastic stresses are the driving force for such behavior.
3.2. Infinitely long cylinders (no side-walls)

We first analyze the flow of a Newtonian fluid through an infinite array of cylinders. This case has been studied in the literature [17] and we find very similar observations. Due to the small spacing between the two cylinders we observe the onset of a recirculation region between the two cylinders, which is actually situated between the front and rear stagnation points of the cylinders. The vortices are counter rotating, which signifies a highly shear dominated flow in this region. The velocity contours and streamlines are shown in figure 8(a) and 8(b).

![Figures 8. (a) Normalized velocity profile and (b) velocity streamlines showing counter rotating vortices for a Newtonian fluid.](image)

Next we analyze the flow of a viscoelastic fluid through the same geometry. The streamlines, colored with the normalized velocity, are shown in figure 9. The simulations clearly show that with an increase in De number \( \text{De} = \frac{\tilde{\lambda}U}{R_c} \) the counter-rotating vortices starts to move away from the centerline of symmetry. It is also very important to observe that up to De number 0.75 the recirculation pattern between the cylinders does not significantly change, but from De number 0.75 onwards the vortices start to become more concave with an increased curvature towards the downstream cylinder compared to the upstream cylinder. The observed streamline patterns are in close agreement with the simulations of Liu et al. [11].
Figure 9. Velocity streamlines (colored with normalized velocity) for viscoelastic fluid at different De numbers.

The normal stress component along the flow direction ($\tau_{xx}$) is shown in figure 10. We observe that with increasing De number this normal stress component gradually increases. The normal stress generation is mostly confined to an angle of 60 to 90° compared to the axis of flow. The largest normal stress is present at the wall of the cylinder, which is mostly shear dominated.

Figure 10. Normal stress ($\tau_{xx}$) profiles for viscoelastic fluid at different De numbers.

The shear stress component $\tau_{xz}$ is shown in figure 11. We observe that with increasing De number the shear stress increases, especially on the upflow surfaces of the cylinders. Similar behavior is found in figure 12, where the normal stress component perpendicular to the flow direction ($\tau_{zz}$) is shown. All other stress components are very small, as expected for this geometry.

Figure 11. Shear stress ($\tau_{xz}$) profiles for viscoelastic fluid at different De numbers.
3.3. Confined cylinders (side-walls)

Now we turn to the second case with side-walls. First we studied the flow of a Newtonian fluid. In comparison to the flow without side-walls we observed a very similar pattern of streamlines of the velocity field in the central plane between the two walls ($y=0$). We observe a small decrease in the size of the counter rotating vortices at a distance of $+R_c$ and $-R_c$ from the center plane, as shown in figure 14. This small change is caused by the reduced velocity induced by friction with the solid walls.
Finally, we investigate the flow of a viscoelastic fluid in the presence of side-walls. Figure 15 shows the streamlines, colored with the normalized velocity in the central $y=0$ plane. Perhaps surprisingly, we find a very large difference in the flow behavior compared to the case without side-walls (or a Newtonian fluid with side-walls). The onset of flow asymmetry is greatly enhanced by the presence of side walls: we observe that already after $De=0.25$ the eyes of the counter rotating vortices start to move away from the centerline of symmetry. Apart from this asymmetry in the $xz$-plane, a secondary flow is also observed in the $xy$-plane (not shown).

The elastic instability is observed through visual inspection. The counter rotating vortices loses symmetry after a $De$ number around 0.25 in the presence of side walls. With increasing Deborah number the polymers do not get sufficient time to relax. The eye of the vortices shift away from the central $xy$-plane and move in the direction of the flow. This causes a loss of symmetry along the central $yz$-plane. We locate the onset of the instability by plotting the displacement of the eye of the counter rotating vortex starting from the central $xy$-plane (i.e. along the $z$ direction) as a function of $De$ number (Figure 16).
Figure 16. Location of the eye of the vortex along the z direction with increasing De number (x-axis normalized w.r.t cylinder radius $R_c$) in the presence of side walls.

We observe that the eye of the counter rotating vortex lies at $0.367R_c$ at De of 0.01. The eye of vortex steadily moves upwards with increasing De number, but after De 0.25 a significant movement of the vortex to $0.48R_c$ is observed. Beyond De 0.50 the vortex location does not change significantly anymore. Apart from the upward motion, the vortex also moves along the flow (x) direction with increasing De number, which follows similar behavior (not shown here). Besides this, as we will show below, a pronounced flow in the y-direction develops. Our observations match closely with the critical De number predicted by the correlation of Smith et al [14] (without wall effects).

Figure 17. Normal stress profiles ($\tau_{yy}$) in the plane $z = 0$ without side-walls and with side-walls at different De numbers.

If we compare the overall viscoelastic stress profiles with the previous case without side-walls, the normal stress components $\tau_{xx}$ and $\tau_{zz}$ are very much comparable (not shown). However the $\tau_{yy}$ component, which is essentially zero without side walls, becomes very significant in the presence of side-walls. The stress profiles in figure 17 show that this stress component is high at the side walls and reaches zero in the center plane between the walls. The magnitude of this
stress component increases with increasing De number. The presence of such stresses may be significant for flow bifurcations and loss of symmetry.

**Figure 18.** 3D representation of direction-vectors (colored with Normal stress ($\tau_{yy}$)) in the plane $x = 0$ with side walls at different De numbers

In figure 18 we show that with increasing Deborah number the velocity vectors increasingly point towards the centre of the domain in the gap between two cylinders. This may be a possible mechanism to explain the elastic instability as also observed by Sahin et al. [42]. The viscoelastic stress ($\tau_{yy}$) affects the streamline curvature which perturbs the velocity components leading to the three dimensional instability.

**Figure 19.** Streamlines showing flow profiles in the $z = 0$ plane: (a) along the Y axis without side walls, (b) along the surface of the cylinder without side walls, (c) along the surface of the cylinder with side walls (flow direction is along $+x$ axis shown by arrow) for De 0.25.

The 3D stream tracers in figure 19 (a) confirm the presence of the counter rotating vortices in between the two cylinders. Figure 19 (b) and (c) shows the stream tracers along the surface of the cylinders. The interesting aspect is that in presence of side walls the stream lines shows an inward motion as explained in figure 18. The vicinity of a subsequent cylinder is responsible for enhancing this effect. Such inward motions are not observed far away from the cylinder surface. This proves that both the cylinder curvature and side walls are responsible for such instabilities.
4. Conclusion

In this paper we show the development of a novel second order immersed boundary methodology to simulate viscoelastic flows in porous media. Until now the use of IBM methods were mostly limited to Newtonian flows. The most important advantage of IBM is its comparatively easier implementation by avoiding body-conforming meshes. It therefore promises to be able to mimic any random flow structure, which is of critical importance for random porous media. We verified the model for the flow past a single cylinder in a channel. The results match well with the previous work of Alves et al. Even at relatively high De numbers of the order 1 we do not encounter any numerical instabilities arising due to pressure and/or high normal stresses. In our implementation we made use of a staggered grid, which decreases the chance of pressure oscillations. This may be critical for viscoelastic flow at high normal stress differences.

We verified our results with the present literature and investigated the flow structures for a highly idealized porous structure made by a periodic arrangement of cylinders. We kept the cylinder spacing very close to study the flow behavior at a relatively strong coupling between the fluid and its confinement. We studied two different cases, with or without side-walls in the direction of the long axis of the cylinders. Although these simulations are computationally expensive, by using periodic boundary conditions and a parallelized code we were able to study the full three-dimensional viscoelastic flow through these geometries for De numbers up to 2.0 and a low Reynolds number (of 0.01).

In all cases counter-rotating vortices appear in between the cylinders. In case of Newtonian flow these vortices are very symmetric around the central axis of flow. For the viscoelastic fluid however we observed a change of vertical structure at higher De number. Without side-walls, the symmetry of the vortices is lost at a De number of approximately 0.75, while with side-walls the critical De number is approximately 0.3. We studied how the velocity and stress profiles are developing in such a complex flow geometry. With side-walls the development of a weak secondary flow across the side-walls was observed. With increasing De number, the normal stress component $\tau_{yy}$ increases significantly. Gradients in this stress component drive the flow velocity to develop components in the direction normal to the side-walls. It will be very interesting to extend our study to flow behavior of viscoelastic fluids in random porous structures in a three dimensional multiphase flow.

5. Acknowledgements

This work is part of the Industrial Partnership Programme (IPP) 'Computational sciences for energy research' of the Foundation for Fundamental Research on Matter (FOM), which is part of the Netherlands Organisation for Scientific Research (NWO). This research programme is co-financed by Shell Global Solutions International B.V.
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