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Assessing OpenFOAM for DNS of Turbulent Non-Newtonian Flow in a Pipe

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Abstract

Transition and turbulence in shear-thinning non-Newtonian fluids are not fully understood yet they can have important application in industrial processes in the chemical, polymer and mineral processing industries. Most existing DNS studies on shear-thinning fluids apply only to simple geometries such as pipes and channels and use bespoke computer codes that are not generally applicable to complex geometries. Therefore, a more generalised DNS approach is needed for modelling turbulence and transition in shear-thinning fluids. The widely used open source CFD library OpenFOAM has recently shown great potential in DNS of turbulent flow. In this study, we conduct benchmark testing on OpenFOAM for DNS of turbulent Newtonian and shear-thinning non-Newtonian flow in a pipe. Results predicted by OpenFOAM for DNS of shear-thinning fluids are assessed by comparing with those obtained by a validated spectral element DNS code Semtex. For Newtonian fluids, we find the mean flow profiles predicted by OpenFOAM correspond very well with Semtex results and experimental data. However, for shear-thinning fluids, OpenFOAM predicts the flow being more transitional with both lower radial and azimuthal turbulence intensities than Semtex results. OpenFOAM does not capture the near wall structure as well as Semtex due to its comparatively lower second-order accuracy and the maximum difference likely to be encountered is in the peak value of turbulence intensities which can be as high as 15%. Despite the lower second order spatial and temporal discretisation schemes applied in OpenFOAM, the study reveals OpenFOAM is still capable to provide reasonably good DNS results in modelling turbulent canonical flow for engineering grade simulations.

Introduction

Non-Newtonian fluids are widely used in industrial processes in the chemical, polymer and mineral processing industries. The flow of non-Newtonian fluid can occur in either laminar or turbulent flow regime due to its moderate viscosity. Compared to laminar flows, turbulent non-Newtonian flows are more complicated to predict. Many non-Newtonian fluids in industrial applications exhibit a shear-thinning behaviour where the viscosity decreases with increasing shear rate. However, transition and turbulence in shear-thinning non-Newtonian fluids are not fully understood yet and require further investigation.

Some experimental work exists on studying the transition and turbulence in non-Newtonian polymer solutions [1]. However, adjusting the rheological properties of laboratory non-Newtonian fluids can be difficult and may bring additional undesirable visco-elastic effect. Compared to experiments, computational modelling has been increasingly applied to modelling transitional and turbulent flow. There have been efforts to evaluate Reynolds-averaged two equation turbulence models for turbulent flow of power-law fluids [2]. The Reynolds-averaged approach is appealing due to its computational convenience but it employs partially empirical parameters that are still lacking for shear-thinning fluids. Molla and Paul [3] performed Large Eddy Simulation (LES) of non-Newtonian blood flow with rheology described using power-law and Casson models, but suitable SGS models for shear-thinning fluids are still poorly developed.

In comparison with the Reynolds-averaged and LES approach, Direct numerical simulation (DNS) is promising in providing detailed information on the transition and turbulence in shear-thinning fluids. Some DNS studies can be found on investigating the drag reduction in turbulent visco-elastic fluids [4]. Ohta and Miyashita [5] conducted DNS of shear-thinning fluids using high-order finite-difference method on structured meshes, but their code only applies to simple geometries like pipes and channels. DNS studies of turbulent shear-thinning flows using the Spectral element—Fourier method (SEM) have also been investigated [6]. Their work revealed the shear-thinning fluids developed larger and weaker turbulent structures compared to a Newtonian fluid at equivalent Re. Despite these work, a generalised DNS approach that could be used to great effect in different flow scenarios is lacking for shear-thinning fluids.

We aim to assess OpenFOAM for DNS of turbulent shear-thinning flow due to its potential to model complex geometries. Recent studies have also shown great promise of OpenFOAM in DNS of turbulent flow [7]. In addition, OpenFOAM code is open source and modularly structured, making it easier for further development. However, very few DNS studies using OpenFOAM focus on shear-thinning fluids, with only some work done in the creeping and laminar flow regimes [8]. In this study, we conduct DNS of turbulent Newtonian and shear-thinning non-Newtonian flow in a periodic pipe using OpenFOAM and compare the DNS results with those from Semtex (a validated spectral element DNS code [9]) to assess OpenFOAM for DNS of shear-thinning fluids.

Non-Newtonian rheology

Rheology Model

The non-Newtonian rheology of the fluid is described with a generalised Newtonian (GN) model, where the fluid stress tensor is the product of an isotropic viscosity and the rate-of-strain tensor,

$$\tau_{ij} = \eta(\dot{\gamma}) S_{ij} \tag{1}$$

The viscosity η is dependent on a shear rate, $\dot{\gamma}$ defined as the second invariant of the rate-of-strain tensor

$$\dot{\gamma} = \left(2 \textstyle\sum_{i,j} S_{ij} S_{ji}\right)^{1/2} \tag{2}$$

The generally used Herschel–Bulkley (HB) model is selected here with viscosity expressed as

$$\eta = \frac{\tau_Y}{\dot{\gamma}} + K\dot{\gamma}^{n-1} \quad (3)$$

where K is the consistency, n is the flow index, and τ_Y is the fluid yield stress.

Generalized Reynolds Number

Defining the Reynolds number in a non-Newtonian flow can be difficult due to the spatially and temporally changing viscosity. A number of options for wall bounded flow have been discussed and the option of mean wall viscosity η_w is selected here[6]. For a HB fluid, the mean wall viscosity can be obtained as

$$\eta_w = \frac{K^{1/n}\tau_w}{(\tau_w - \tau_Y)^{1/n}} \quad (4)$$

where τ_w is the mean wall shear stress. With a given pressure gradient $\partial P/\partial Z$, τ_w can be calculated as

$$\tau_w = \frac{D}{4}\frac{\partial P}{\partial Z} \quad (5)$$

where D is the pipe diameter. By replacing the Newtonian viscosity with the mean wall viscosity, the generalized Reynolds number is obtained as

$$Re_G = \frac{\rho U D}{\eta_w} \quad (6)$$

Numerical Methods

General

Non-dimensional units are used in this paper for the results analysis. The friction velocity U_τ is calculated as:

$$U_\tau = \sqrt{\frac{\tau_w}{\rho}} \quad (7)$$

thus, the non-dimensional velocity is defined as

$$U^+ = \frac{U}{U_\tau} \quad (8)$$

Similar to define the generalized Reynolds number in the previous section, with the mean wall viscosity replacing the constant Newtonian viscosity, wall units in a non-Newtonian pipe flow are presented as

$$y^+ = \frac{\rho U_\tau}{\eta_w}(R - r) \quad (9)$$

where R is the pipe radius, r is the radial distance from the pipe center.

Governing Equations

Since incompressible Newtonian and shear-thinning non-Newtonian flows are considered in this study, the kinematic viscosity $\nu = \frac{\eta}{\rho}$ is used. Both flows can be described with the following conservation equations of mass and momentum (without gravity),

$$\nabla \cdot \boldsymbol{U} = 0 \quad (10)$$

$$\frac{\partial \boldsymbol{U}}{\partial t} + \nabla \cdot (\boldsymbol{U}\boldsymbol{U}) = -\nabla p + \nabla \cdot (\nu \nabla \boldsymbol{U}) \quad (11)$$

For the shear-thinning flow, ν is described with the Herschel–Bulkley model (equation 3).

Implementation In OpenFOAM

A periodic pipe with length of $4\pi D$ is studied and the entire computational domain is discretized with structural hexahedral elements using ICEM-CFD. Table 1 shows the details of the three different mesh resolutions used. Meshes are uniform in the axial direction and a meshing-spacing ratio is applied in the radial direction with 36 layers generated in the near-wall region (r/R>0.55). Figure 1 displays the cross-sectional view of the mesh (4.1 million). The other two meshes are qualitatively similar.

Mesh Resolution	Coarse	Medium	Fine
Number of cells	1.4	4.1	8.0
r^+, $(R\theta)^+$ and z^+	1.0,9.4,14.1	0.5,5.7,9.4	0.5,4.7,5.7

Table 1. Details of the computational domain discretization

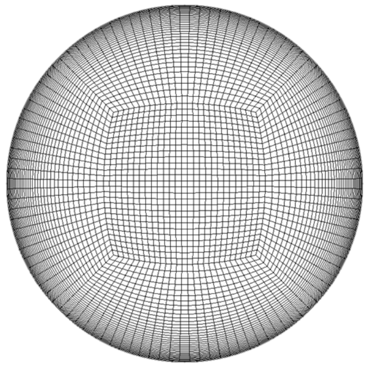

Figure 1. Cross-section view of the meshes (4.1million)

Newtonian simulations are initialized with a perturbed laminar flow whereas the fully developed Newtonian flow is used as an initial condition for shear-thinning fluid. In terms of the boundary conditions, the flow is periodic in axial direction with standard no-slip condition applied at the pipe wall. A corresponding body force per unit mass equivalent to the pressure gradient of the flow is applied to the z-momentum equation for periodic pressure implementation.

To ensure the flow reaches a statistically steady state, 10 Flow Through Times (FTT=L/$\overline{U}$) are normally required after initialization. Afterwards, simulations continue for another 30 FTTs to accumulate turbulence statistics. Simulations are conducted using Cartesian coordinates and results have been transformed into cylindrical coordinates, with homogeneous averaging done in both axial and azimuthal directions for final analysis of mean quantities.

All simulations are conducted with OpenFOAM v4.1. The DNS of Newtonian and shear-thinning flows are solved with IcoFoam and nonNewtonianIcoFoam solvers, respectively. PISO algorithm is used for the pressure-velocity coupling. All the spatial discretization schemes used are of second-order accuracy and backward scheme is used for the time discretization. Pressure is solved with the Pre-conditioned Conjugate Gradient (PCG) solver and velocity is solved with the smoothSolver with a corresponding symGaussSeidel smoother.

Implementation In Semtex

Semtex is a spectral element simulation code developed by Blackburn and Sherwin [9] and has been validated for DNS of incompressible flow. In the spectral element method, the computational domain is discretized into two-dimensional isoparametrically mapped quadrilateral spectral elements, with a third orthogonal direction for the Fourier expansions. More information regarding Semtex can be found in [9].

In Semtex, the pipe studied is of the same length $4\pi D$. For the discretization of the computational domain, 161 9th-order elements in the cross-section and 192 Fourier modes in the axial direction are applied, with a total number of grid nodes 2.6 million. The cross-section of the mesh in Semtex is shown in Figure 2. The resolution used has been demonstrated to give converged results in [6]. The near-wall mesh resolution is $r^+ \approx 0.85$, $(R\theta)^+ \approx 4.8$ and $z^+ \approx 22.4$. Turbulence statistics are accumulated for 30 FTTs after reaching statistically steady state. To ensure periodic pressure implementation, a body force equal to the pressure gradient is applied in the axial momentum equation.

Simulation Parameters

A shear-thinning flow can become turbulent or transitional due to its moderate viscosity. This study mainly focuses on transitional or weakly turbulent flow of shear-thinning fluids. Therefore, a Reynolds number of 5000 is used for both Newtonian and shear-thinning flow. Table 2 shows the parameters used for the Newtonian and shear-thinning flow in OpenFOAM (OF) and Semtex.

Sim.	$\partial p/\partial Z$	τ_Y	K	Predicted Re_G	
				OF	Semtex
Newt	0.188	N/A	N/A	5011	4992
HB	0.148	6.62e-05	1.22e-04	5018	4757

Table 2. Non-dimensional parameters for the simulations (Note: the non-dimensionalised pipe diameter is 0.1; Expected superficial flow velocity is 1; n=0.65)

Blasius correlation is used to calculate the pressure gradient for Newtonian flow. For HB fluids, the Wilson and Thomas correlation [10] is applied to obtain the expected pressure gradient for given rheological parameters.

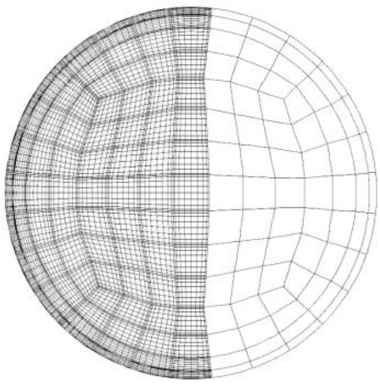

Figure 2. The pipe cross-section mesh in Semtex (Left: nodal points; Right: underlying spectral mesh)

Results

Velocity and Viscosity Contours

Instantaneous velocity contours for both Newtonian and shear-thinning fluids and viscosity contours for shear-thinning fluids are shown in Figure 3. The viscosity is non-dimensionalised with the mean wall viscosity.

The velocity and viscosity contours predicted by Semtex and OpenFOAM are qualitatively similar and reveal the level of turbulence development in Newtonian and shear-thinning flow. There is a distinct difference between the Newtonian and shear-thinning velocity contours that random and small-scale turbulence structures are found in the Newtonian flow, while a less convoluted, large-scale structure is observed in the shear-thinning flow. The viscosity contours show an obviously higher viscosity in the center of the pipe than in the near wall region. This high viscosity in the core will dampen the momentum transfer in the radial direction, giving rise to a more transitional flow.

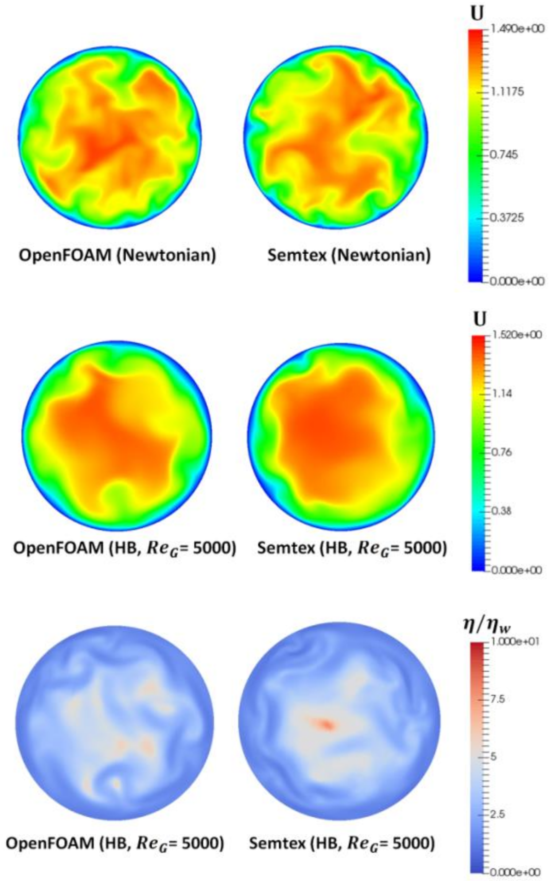

Figure 3. Velocity and viscosity contours for simulations

Mean Flow Profiles of Newtonian Fluids

The mean and turbulence intensity profiles of Newtonian and HB fluids are shown in Figure 4 and Figure 5, respectively. This section compares the DNS results of Newtonian flow predicted by OpenFOAM and Semtex. Note that three different resolutions as described in the meshing section have been used for the simulations and the 4.1 million has been demonstrated to be sufficient for the current studies (results not shown here).

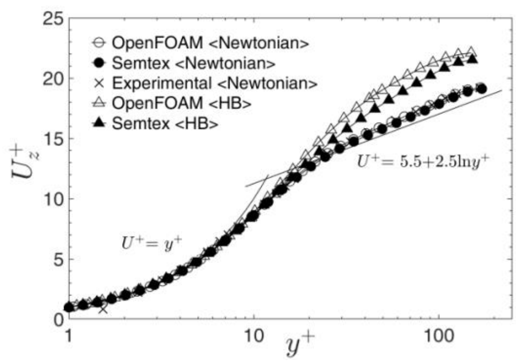

Figure 4. Mean velocity profiles for the turbulent pipe flow

As shown in Figure 4, the mean velocity profile of Newtonian fluid predicted by OpenFOAM matches very well with the Semtex results and experimental reference, with only a slight difference within 0.6% when comparing the peak value of the OpenFOAM solution with the Semtex solution. Both profiles correspond well with the conventional 'Law of the wall', where U^+ varies linearly with y^+ in the near wall region and follows the log-law relationship ($U^+ = A + B\ln y^+$) in the log region. A higher A of 5.5 instead of the commonly used value of 5.0 is used to better represent turbulent flow with low Reynolds number, which is the case in this study.

As can be seen in Figure 5, all the turbulence intensities and Reynolds shear stress profiles of Newtonian fluids correspond very well, with OpenFOAM slightly underpredicting the turbulence intensities. The differences for the axial, radial and azimuthal intensity are only 1.1%, 4.1% and 3.0%, respectively when comparing the peak value with Semtex results. The results indicate OpenFOAM is reliable for DNS of turbulent Newtonian flow and provides satisfactory results of the mean flow profiles compared to other DNS references. The maximum difference found for Newtonian flow in this study is 4.1% when predicting the radial turbulence intensity.

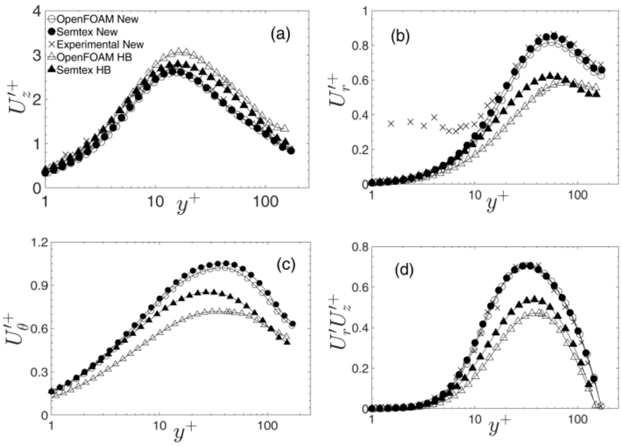

Figure 5. The turbulence intensity and Reynolds shear stress profiles (a) axial, (b) radial, (c) azimuthal and (d) Reynolds shear stress

Mean Flow Profiles of Non-Newtonian Fluids

The mean flow profiles of the HB fluid are also displayed in Figure 4 and Figure 5. The mean velocity profiles of HB fluid lie slightly above the plotted conventional 'Law of the wall' non-dimensionalisation, indicating the flow predicted to be more transitional compared to an equivalent Newtonian flow. OpenFOAM predicts the flow to be even more transitional as its velocity profile lies above the corresponding Semtex profile. The velocity profiles of HB fluid match very well in the near wall region but start to deviate in the log and core region. The difference at the peak for HB fluid is 2.7%.

The turbulence intensities of HB fluid also suggest the flow predicted with OpenFOAM is more transitional with higher axial intensity but lower radial and azimuthal intensity. The differences between OpenFOAM and Semtex in axial, radial and azimuthal turbulence intensities are 10.0%, 5.9% and 15.7%, respectively when comparing the peak values. The Reynolds stress predicted with OpenFOAM also lies below the Semtex profile with an approximately 12.5% difference at the peak for the HB fluid. These differences are very large compared to those seen for Newtonian fluid.

The turbulence intensity profiles of HB fluid indicate OpenFOAM doesn't capture the near wall structure as well as Semtex. Semtex adopts the higher order spectral element-Fourier method, while OpenFOAM adopts relatively lower second-order spatial and temporal discretisation schemes. In addition to the discretisation scheme effects, DNS of HB fluids may require higher mesh resolution due to its non-uniform viscosity, despite the 4.1 million mesh resolution is sufficient for Newtonian flow. Further studies will be conducted with a higher mesh resolution by refining the meshes, particularly in the azimuthal direction (where the maximum difference lies). Considering the high viscosity of the HB fluid with Re_G=5000, the turbulent flow field remains mostly transitional and not fully developed. DNS of shear-thinning flow with a higher Re_G will also be carried out to assess OpenFOAM for DNS of shear-thinning flow. Preliminary simulations suggest the differences between Semtex and OpenFOAM predictions decrease at higher Reynolds number. Details are not revealed here due to the limited space in this paper. Results of HB fluid with Re_G=5000 reveals OpenFOAM predicts the shear-thinning flow profiles within a few percent of the Semtex references, the maximum difference likely to be encountered is in the peak value of turbulence intensities which can be as high as 15%.

Conclusions

The current paper aims to assess a more generalised DNS approach for shear-thinning non-Newtonian fluids by using OpenFOAM. We conduct DNS of turbulent Newtonian and shear-thinning flow in a periodic pipe and compare the results with a validated DNS code Semtex. We find OpenFOAM is reliable for DNS of turbulent Newtonian flow and provides satisfactory results of the mean flow profiles; while for shear-thinning fluid, OpenFOAM predicts the flow being more transitional with both lower radial and azimuthal turbulence intensities and the maximum difference likely to be encountered is in the peak value of turbulence intensities which can be as high as 15%. OpenFOAM provides reasonably good DNS results in modelling turbulent canonical flow for engineering grade simulations despite its lower second-order accuracy. Considering the turbulent shear-thinning flow of HB fluid with Re_G=5000 being not fully developed in this study, further investigations on DNS of turbulent shear-thinning flow with higher Re_G will be conducted.

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