Non Newtonian transport in OpenFOAM: validation and applications

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Abstract. Most of the fluids used in all industries nowadays can be classified as non-newtonian. In numerical simulations conducted via Computational Fluid Dynamics (CFD) techniques, as a consequence of its highly non-linear behavior, this kind of material is usually described by a mathematical model. The way this model represents the fluid affects immensely the manner it flows in a domain, and the correct transport model can increase precision and detail capturing of a simulation. The purpose of this work is to validate the Herschel-Bulkley rheology model, implemented in the CFD open source tool OpenFOAM, reproducing experimental conditions and comparing results with benchmark data. To this end, the cases chosen for study all involved non-newtonian fluids, and are extensively researched problems in civil engineering. Furthermore, it is presented an application of rheology in CFD in the investigation of blood flow in the aortic arch. Four different rheology models are used to simulate blood behavior, Carreau, Casson, Cross and Power Law.

Keywords: computational fluid dynamics (CFD), rheology, non newtonian fluids.

1 Introduction

Non newtonian fluid behavior is a complex and highly nonlinear phenomena that occurs in materials present in various fields nowadays, from civil engineering (Sant [1]; Cremonesi [2]) and construction to medical engineering and hemorheology (Secomb [3]). Computational Fluid Dynamics (CFD) has proven to be a very useful and reliable tool in those fields, however modeling such non newtonian behavior numerically can be challenging (Batchelor [4]; Hirsch [5]), since its viscosity varies along time and space obeying a certain function, established by a rheology model that has to be chosen when running CFD simulations. Given the complex behavior of those fluids, choosing such a rheology model that can best predict its flow can be challenging. Several models are used in different CFD codes, however, the majority of commercially available software options provide users with only a limited range of choices when it comes to modeling viscous fluids. OpenFOAM, on the other hand, is an open source CFD tool that provides the user the option between five of the traditional non-newtonian rheology models for complex fluid dynamic analysis, while also giving the user the possibility to implement other rheology models.

CFD techniques have been used in a series of problems due mainly to the relatively low cost of simulations in comparison to experimental tests, and precision of results obtained. In order to validate the OpenFOAM transport model utility that predicts non-newtonian fluid flow, a benchmark case was chosen: the dam break problem. The fluid was modeled as a Bingham plastic, using the implemented Herschel-Bulkley model, and the parameters obtained from experimental data. With regards to cases of hemodynamics, experimental data cannot be obtained without expensive and invasive procedures. Furthermore, rheology assumes a particularly important role in hemodynamic studies due to the influence of viscosity in wall shear stress (WSS) and fluid-structure interaction analysis (Yilmaz [6]). Several studies have tried to determine the rheology model that best describes blood behavior (Carvalho [7]; Wajihah [8]). Moreover, owing to the extraordinarily complex geometry of blood vessels, some regions have blood flowing at low velocities, causing the viscosity's influence in the flow to increase (Crochet [9]). The correct modeling of blood's rheological properties can increase precision of CFD simulations and reliability of results, therefore offering a database that can serve as basis for decision making and assist medics in patient-specific cases, design of medical devices and even prevention of diseases related to the cardiovascular system. Thus, in this work the authors conducted a validation case and investigated the influence of rheology models in the results of blood flow through an FDA nozzle and an aortic arch.

2 Mathematical formulation

2.1 Governing equations

OpenFOAM is a mesh based CFD tool that solves the conservation equations using the Finite Volume Method (FVM) and volume of fluid (VOF). For the simulations conducted for this paper, the fluid was always considered incompressible, and heat transfer was not considered in any of the simulations. Thus, the governing equations used were those of mass (continuity) and momentum (Navier-Stokes) conservation, given below.

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

$$\frac{\partial u_i}{\partial t} + \frac{\partial (u_i u_j)}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_i}\left(\mu \frac{\partial u_i}{\partial x_j}\right) + f_i$$

Where u is the velocity component, t is time, ρ is the mass density, p is the pressure, μ is the dynamic viscosity, and f represents possible external forces.

2.2 Rheology models in OpenFOAM

The solvers models viscosity following the five classical rheology models as presented below.

Table 1. Rheology models formulation in OpenFOAM

Rheology/Transport Model	Kinematic Viscosity
Bird-Carreau	$\nu = \nu_\infty + (\nu_0 - \nu_\infty)[1 + (k\gamma)^a]^{\frac{(n-1)}{a}}$
Power Law	$\nu = k\gamma^{n-1}$
Cross Power Law	$\nu = \nu_\infty + \frac{(\nu_0 - \nu_\infty)}{1+(m\gamma)^n}$
Herschel-Bulkley	$\nu = min\,(\nu_0, \tau_0/\gamma + k\gamma^{n-1})$
Casson	$\nu = (\sqrt{\tau_0/\gamma} + \sqrt{m})^2$

3 Validation

3.1. Dam break (Carbopol 940)

The dam break problem is extensively investigated as a troubleshooting technique in many CFD studies (Hu [10]). Aiming to validate the Herschel-Bulkley model, a dam break simulation model was reproduced with a Carbopol 940 fluid column, a non newtonian polymer that behaves as a Bingham plastic. The Bingham behavior can be modeled through the Hershcel-Bulkley equation from Table 1 using the following parameters.

Table 2. Coefficients in Herschel-Bulkley for Carbopol 940

τ_0 [Pa]	K [Pa.s^n]	n
4.4715	1.1849	0.5497

The results obtained from OpenFOAM were compared with numerical results from Freeflow, a simulation software based on finite differences method, which were previously validated using experimental results (Leite [11]). The mesh used for this case was generated in the OpenFOAM tool blockMesh, consisting of 300x40 regular 0.005 meters squares, and the simulation was conducted in the implemented interFoam multiphase solver.

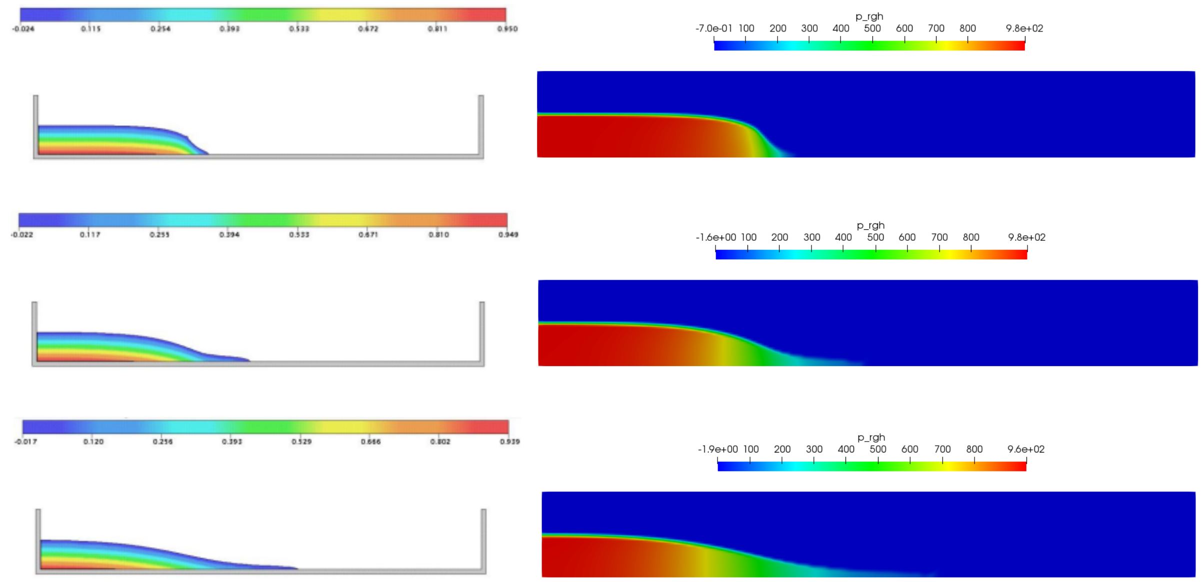

Figure 1. Pressure fields in Freeflow (left) and OpenFOAM (right) through times 0.1, 0.2 and 0.3s

4 Application

4.1. Benchmark nozzle (FDA)

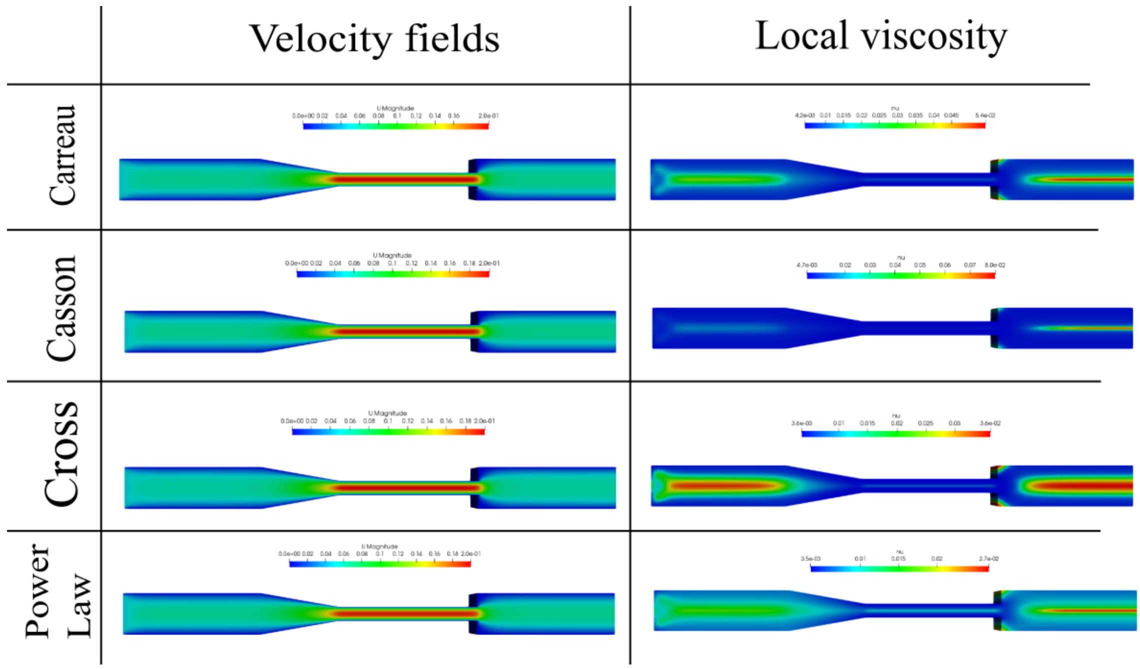

Figure 2. Velocity fields and local viscosity at 15s

For this first application, data for geometry and boundary conditions was obtained from (Raben [13]) and (Zakaria [14]), in which experimental and numerical simulations were conducted, respectively, inside an artificial coronary nozzle designed by the American Food and Drugs Administration (FDA). In order to model blood behavior, four of the transport models implemented in OpenFOAM were applied to this case, for which parameters were used following those gathered by Chen [15].

Given the preliminary results shown in Figure 2, blood properties modeled using different rheology equations can bring about significantly different responses. Future work will evaluate the impact the rheology model has in wall shear stress (WSS) values, and how it affects the blood vessels' wall and tissues.

4.2. Aortic arch

Lastly, the same transport models were applied in a domain with complex geometry, related to applications in hemodynamics, which is the focus of this study. To this last application, the aortic arch was chosen due to its importance in the human body. The model considered the outlets as fixed pressures, and in future work being currently developed by the authors the modeling of outlet boundary conditions will include Windkessel lumped models and Murray's Law. Blood properties used for this case are the same as used in the nozzle case.

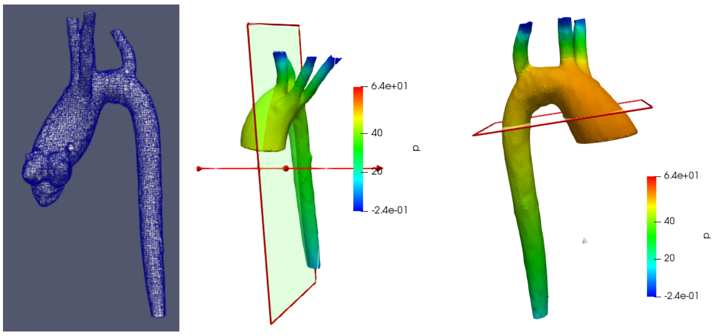

Figure 3. Aortic arch case mesh and domain

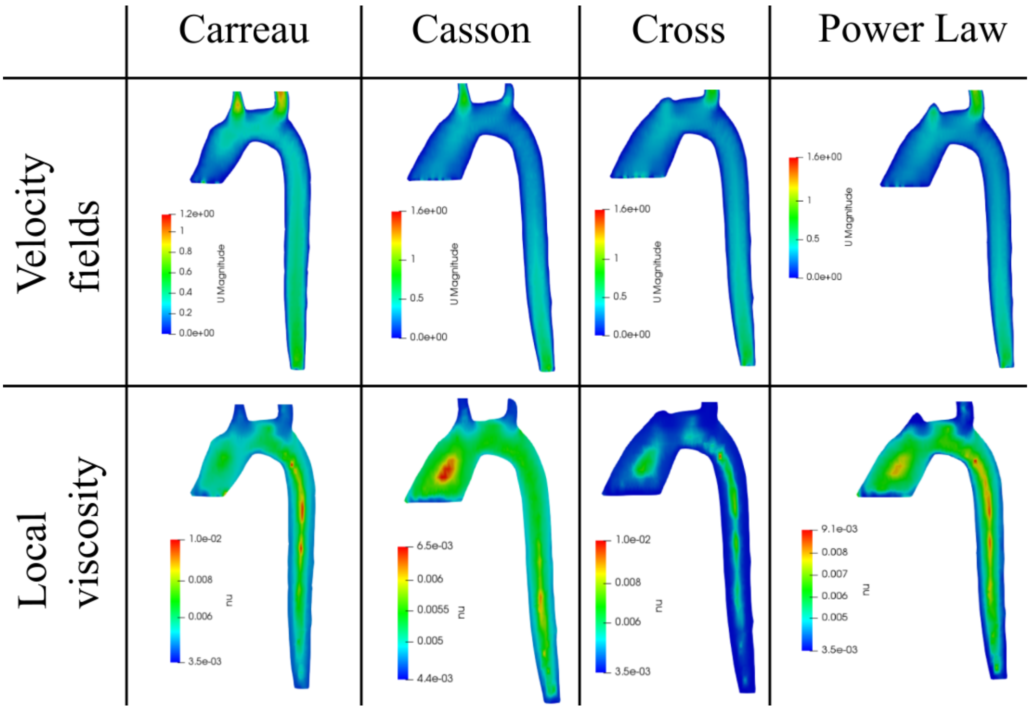

Figure 4. Velocity fields and local viscosity at 15s

Preliminary results can show that the rheology model selected for the hemodynamics simulations can change the values of local viscosity, which can lead to different values of wall shear stress and velocities. Locating with precision the regions where there is significant increase in local viscosity can prevent coagulation and energy loss in the flow. While the local viscosity value can have little to no effect on high velocity flow, such as in the aorta, its effect can be determinant to understanding smaller scale cases, for example as studied by Abazari [15] in a type-B aortic dissection, disease for which there is no recommended treatment, and each case must be studied separately, using for example high precision CFD simulations as a non invasive option for obtaining data.

5 Conclusions

The validation test case performed showed that the Hershel-Bulkley model implemented in OpenFOAM produced results that agreed with the data previously obtained in FREEFLOW, and the experimental results from Leite [11]. From the partial results obtained until now, the authors found that the rheology model selected can largely impact the values for local viscosity, and therefore the wall shear stress (WSS) and fluid-structure interactions. Further work will explore different rheology models under non-traditional boundary conditions, and its effect on WSS and blood flow.

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