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TOPOLOGY OPTIMIZATION METHOD APPLIED TO DESIGN CHANNELS FOR NON-NEWTONIAN FLUID FLOW

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Abstract. *The present work proposes the study of design channels for steady, incompressible non-Newtonian flow, by using Topology Optimization Method. This study focusses on fluidics systems dealing with blood, and presents itself as relevant when applied to design of biomedical devices such as arterial bypass grafts. The fluid flow is modeled with the Navier-Stokes equations coupled with Carreau-Yasuda constitutive equation for the shear rate dependent dynamic viscosity to take into account the effects of non-Newtonian blood properties. The Topology Optimization Method distributes regions of solid and fluid, given a volume constraint, within a specified domain in order to obtain a geometry and layout that minimizes energy dissipation, by using the material pseudo-density as design variable. To apply this method to fluidic systems design, a fictional porous flow based on Darcy equation is introduced and material interpolation functions for the inverse permeability and dynamic viscosity are defined. The flow model is implemented in its discrete form by using Finite Element Method through the OpenSource platform FEniCS, applied to automate the solution of mathematical models based on differential equations, and the optimization problem is solved by usign the platforms DOLFIN-adjoint and PyIpopt optimizer. Optimal topologies of bidimensional channels for non-Newtonian flow are presented to illustrate the proposed method.*

Keywords: *topology optimization, non-Newtonian fluids, blood flow*

1. INTRODUCTION

Computational Fluid Dynamics (CFD) applied to fluid systems dealing with blood flow has been an active area of intensive research. Motivated by problems in biomedical engineering, many studies aim to model the non-Newtonian effects in blood flow (BOYD, BUICK e GREEN, 2007), (ZAUSKOVA e MEDVID'OVA, 2010) in order to obtain more accurate results, allowing the minimization of blood cells damages in artificial flows.

Numerical optimization procedures based in CFD present various advantages when compared to the traditional trial and error method, thus, many approaches for the design of non-Newtonian fluidic systems have been developed. Most of applications found in literature focus in applying the method of shape optimization (ABRAHAM, BEHR e HEINKENSCHLOSS, 2005), (SOKOLOWSKI e STEBEL, 2013).

Shape optimization solutions do not allow exploring differente configuration of channels, such as two channel topologies. The solutions found through this optimization method are extremely dependent of the initial system configuration. An alternative to overcome this limitation is the topology optimization method (BENDSøE e SIGMUND, 2003), that allows solutions not "intuitive" to appear, through free distribution of fluid or solid in a domain, aiming to minimize or maximize a given objective function.

The implementation of topology optimization method to fluid systems was first introduced by Borrvall e Peterson, and applied to two-dimensional flow channel design, modeled by steady state Stokes flow with negligible inertial effects (BORRVALL e PETERSON, 2003). Since then, the theme has been deeply explored, with studies that focus mainly in Newtonian fluid flow (KOGA, 2010).

Recently, researchers have shown interest in applying the topology optimization method to devices conducing blood, considering viscoelastic effects existent in non-Newtonian fluids. There are approaches that model the fluid flow through the Navier-Stokes equations, as proposed by (HYUN, WANG e YANG, 2014), and also through the Lattice Boltzmann method (PINGEN e MAUTE, 2010), and compare the optimal solutions with the solutions obtained for Newtonian fluids.

In this work, a topology optimization method for designing channel of steady incompressible non-Newtonian fluid flow is presented, by using the software collection FEniCS. It is studied the finite element method to solve the Navier-Stokes equations coupled with the Carreau-Yasuda viscosity model and the optimization of two-dimensional channels that aim to minimize the fluidic system power dissipation.

This paper is organized as follows. In Section 2, non-Newtonian fluid flow modeling is discussed. In Section 3, the topology optimization problem formulation is defined, and the adopted material model is explained. Section 4 briefly shows the numerical implementation, presenting the finite element method and optimization algorithm. Numerical results are discussed in Section 5, and concluding remarks are provided in Section 6.

2. FLUID FLOW MODELING

The flow studied in this work is assumed to be laminar and incompressible. The system dimensions are much larger than blood cells, so that the Navier-Stokes fluid flow model based on continuous assumption can be employed. This fluid flow model is given by the following mass conservation and momentum equations, respectively.

$$\rho_m(\mathbf{u}\cdot\nabla\mathbf{u}) = -\nabla p + \nabla\cdot 2\mu\varepsilon(\mathbf{u}) + \mathbf{f} \tag{1}$$

$$\nabla\cdot\mathbf{u} = 0 \tag{2}$$

where ρ_m is mass density constant through the domain, $\mathbf{u}$ is the velocity field, p is the pressure, μ is the fluid dynamic viscosity, $\mathbf{f}$ are field forces and $\varepsilon(\mathbf{u})$ is the rate-of-strain tensor given by

$$\varepsilon(\mathbf{u}) = \frac{1}{2}\left(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}\right) \tag{3}$$

In the optimization problem is it necessary to control the distribution of solid and fluid regions within a domain, so a mixed model for fluid flow through a porous medium (BORRVALL e PETERSON, 2003), known as Darcy's law, has been applied

$$\alpha\mathbf{u} = (\nabla \mathrm{p} - \mathbf{f}) \tag{4}$$

where α is the inverse permeability of the porous medium.

The Navier-Stokes equations and Darcy's Law are combined by using the Brinkman equations (CITAR), which allow the use of both models in a single system equation, thus, the final system is represented as follows

$$\rho_m(\mathbf{u}\cdot\nabla\mathbf{u}) = -\nabla \mathrm{p} + \nabla\cdot 2\mu\varepsilon(\mathbf{u}) + \mathbf{f} - \alpha\mathbf{u} \tag{5}$$

$$\nabla\cdot\mathbf{u} = 0 \tag{6}$$

2.1 Non-Newtonian Flow

For a Newtonian fluid, the dynamic viscosity μ is constant, whereas in non-Newtonian fluids this property depends on the fluid shear rate $\dot{\gamma}$, which is given by

$$\dot{\gamma} = \sqrt{2\varepsilon(\mathbf{u}):\varepsilon(\mathbf{u})} \tag{7}$$

Blood is a non-Newtonian fluid that displays the shear thinning effect, i.e., the viscosity decreases with an increased shear rate. In this work, the Carreau-Yasuda model was used to describe this behavior of blood, which has a viscosity function given by

$$\mu(\dot{\gamma}) = \mu_\infty + (\mu_0 - \mu_\infty)\left[1 + (\lambda\dot{\gamma})^a\right]^{\frac{n-1}{a}} \tag{8}$$

where μ_∞ is the infinite shear viscosity, usually defined as the Newtonian viscosity, μ_0 is the zero shear viscosity and λ, a, n, are fluid parameters used to adjust the model.

3. TOPOLOGY OPTIMIZATION PROBLEM

3.1 Material Model

The objective of the optimization problem is to find which regions will be fluid and which will be solid, in order to minimize the power dissipation. A material model is necessary to relax the problem and allow a continuous transition between solid and fluid. In the adopted material model, the design variable is pseudo-density ρ, $0 \le \rho \le 1$ which represents the amount of fluid present at each element of the domain. The material model represents a porous that allows a continuous transition between these two states, through the inverse permeability term. Also, the non-Newtonian effects are reduced in areas of high porosity in order to avoid convergence problems, as proposed by (PINGEN, MAUTE, 2010).

As the final result of the optimization process, the design variable should achieve discrete values so that ρ = 1 represents a pure non-Newtonian fluid and ρ = 0 indicates a fully solid material. In order to suppress the intermediate values of the pseudo-density ρ, non-linear interpolation functions are adopted for describe the inverse permeability and the dynamic viscosity as functions of ρ (HYUN, WANG e YANG, 2014), given by

$$\alpha(\rho) = \alpha_f + (\alpha_s - \alpha_f).\frac{q(1-\rho)}{q+\rho} \tag{9}$$

$$\mu(\rho) = \mu_f + (\mu_s - \mu_f).\frac{q(1-\rho)}{q+\rho} \tag{10}$$

where q is the penalty parameter that controls the linearity of the interpolation functions, μ_f is the shear rate dependent viscosity $\mu(\dot{\gamma})$ and μ_s is equal to the Newtonian viscosity (0.0035 Pa.s). The inverse permeability for fluid material is α_f = 0 and for solid material $\alpha_s \rightarrow \infty$.

3.2 Problem Formulation

In this work, the adopted objective function aims to minimize the total energy dissipation of the system. Borvall and Petersson proposed a formulation for the fluidic energy dissipation that considers the effect of material model, given by

$$\Phi = \frac{1}{2}\int_\Omega \mu(\rho)(\nabla\mathbf{u} + \nabla\mathbf{u}^\mathrm{T}):(\nabla\mathbf{u} + \nabla\mathbf{u}^\mathrm{T})\mathrm{d}\Omega + \frac{1}{2}\int_\Omega \alpha(\rho)\mathbf{u}\cdot\mathbf{u}\mathrm{d}\Omega - \int_\Omega \mathbf{f}\cdot\mathbf{u}d\Omega \tag{11}$$

In addition, a volume constraint is used in a way that, at most, a given fraction of the design domain V is allowed to be occupied by fluid and the remainder must be solid.

$$\int_\Omega \rho\mathrm{d}\Omega \le V \tag{12}$$

Thus, the optimization problem has the following formulation

$$\begin{aligned} &\underset{\rho}{\text{Minimize:}} && \Phi \\ &\text{subject to:} && \int_\Omega \alpha\mathrm{u}\cdot\mathrm{v}\mathrm{d}\Omega + \int_\Omega 2\mu\varepsilon(\mathrm{u})\cdot\nabla\mathrm{v}\mathrm{d}\Omega - \int_\Omega \mathrm{p}(\nabla\mathrm{v})d\Omega = \int_\Omega \mathrm{f}\cdot\mathrm{v}\mathrm{d}\Omega \\ &&& \int_\Omega q(\nabla\cdot\mathrm{u})\,d\Omega = 0 \\ &&& \int_\Omega \rho\mathrm{d}\Omega \le V \\ &&& 0 \le \rho \le 1 \end{aligned} \tag{13}$$

4. NUMERICAL IMPLEMENTATION

4.1 Finite Element Modeling

The partial differential equations presented are solved by using a numerical method since it is very difficult to solve them analytically. The finite element method (FEM) is implemented to find the approximate solution of the Navier-Stokes equations. In order to obtain the weak formulation, the Galerkin's weighted residual procedure is applied.

Thus, the problem weak formulation is given by

$$\int_\Omega \alpha\mathbf{u}\cdot\mathbf{v}d\Omega + \int_\Omega 2\mu\varepsilon(\mathbf{u})\cdot\nabla\mathbf{v}d\Omega - \int_\Omega \mathrm{p}(\nabla\mathbf{v})d\Omega = \int_\Omega \mathbf{f}\cdot\mathbf{v}d\Omega \tag{14}$$

$$\int_\Omega q(\nabla\cdot\mathrm{u})\,d\Omega = 0 \tag{15}$$

where **v** and q are weighting functions, q is scalar and **v** is a vector.

The finite element method is implemented by using the OpenSource FEniCS environment (LOGG, MARDAL e WELLS, 2012), which consists of a collection of software components for automating the solution of PDEs, since it has modules that receive the weak problem formulation and assemble the FEM problem. The library translates a mathematical syntax to a language that can be interpreted by the computer, called DOLFIN, and it also provides various data structures to interface meshes, function spaces, functions and solvers.

The mesh is composed by triangular Taylor-Hood elements, where the velocity has a quadratic interpolation function and the pressure has a linear interpolation. The FEM system is non-linear and non-symmetrical, thus, a more complex solver then the basic Newton method is needed to guarantee the solution convergence. The Multifrontal Massively Parallel Sparse direct Solver (MUMPS) and a preconditioner that is combination of the Incomplete LU factorization (ILU) and Block Jacobi iteration (Bjacobi) have been adopted.

4.2 Optimization Procedure

In order to determine the distribution of fluid and solid material within a design domain, finite element method and an optimization algorithm are combined in an iterative process, described as follows. First, the initial system information (design domain, boundaries) is defined and then the Navier-Stokes equations are solved by finite element method. The value of objective function and constraints are calculated. Then, the functional sensitivities are evaluated and used by an optimizer to update the design variable. This process is repeated until convergence is reached, resulting in the final material distribution. Figure 1 presents the simplified flow chart for the implementation of the topology optimization method.

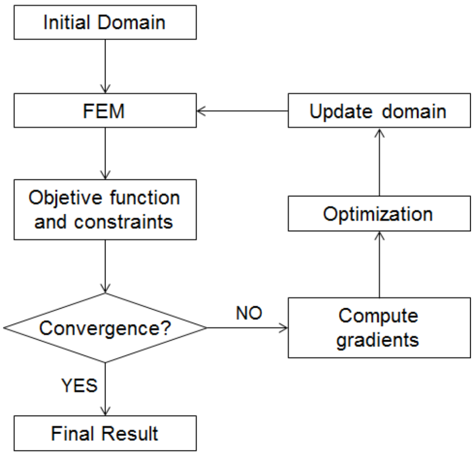

Figure 1. Topology Optimization Implementation Flow Chart

In this work the topology optimization problem is implemented by using the framework formed by the FEniCS system, to solve the PDEs, the libadjoint library, to compute the sensitivities, and the IPOpt optimizer, to update the design variable value. The Internal Point Optimization, implemented through the IPOpt, is a gradient based optimization algorithm will be used, i.e, the direction to update the design variable ρ is given by the gradient information with respect to the chosen functional.

5. NUMERICAL EXAMPLES

In this section, numerical examples are presented to illustrate to proposed methods for non-Newtonian fluid finite element modeling and topology optimization. Blood properties have been adopted in the numerical implementation, where mass density is ρ_m = 1056 kg/m³ and for the Carreau-Yasuda viscosity model, the following values apply (ABRAHAM et al.): a = 0.64, n = 0.2128, λ = 8.2s, μ_∞ = 0.0035 Pa.s and μ_0 = 0.16 Pa.s.

5.1 Validation of Non-Newtonian Finite Element Modeling

The fluid flow over a two-dimensional backward-facing step was analyzed to validate the non-Newtonian fluid model implemented. The results obtained are compared with the literature (SIEBERT, FODOR, 2009) where a case study for different blood viscosity models in COMSOL Multiphysics is presented.

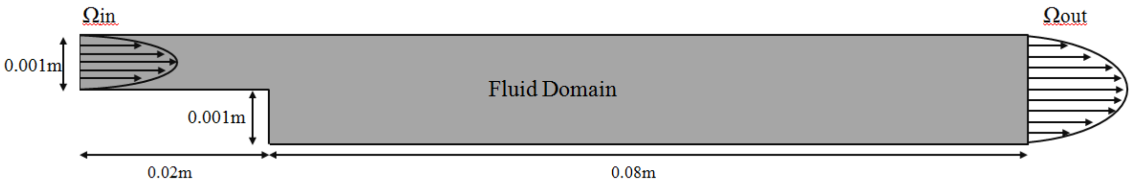

Figure 2. Backward-facing step problem

The influence of inlet maximum velocity (V = 0.025 m/s or V = 0.8 m/s) and the constitutive equation used to model viscosity is show in Fig. 3. The results for Newtonian and Carreau are very similar to those obtained in (SIEBERT, FODOR, 2009). Also, for the viscosity model adopted in this word (Carreau-Yasuda) the results presented the same characteristics.

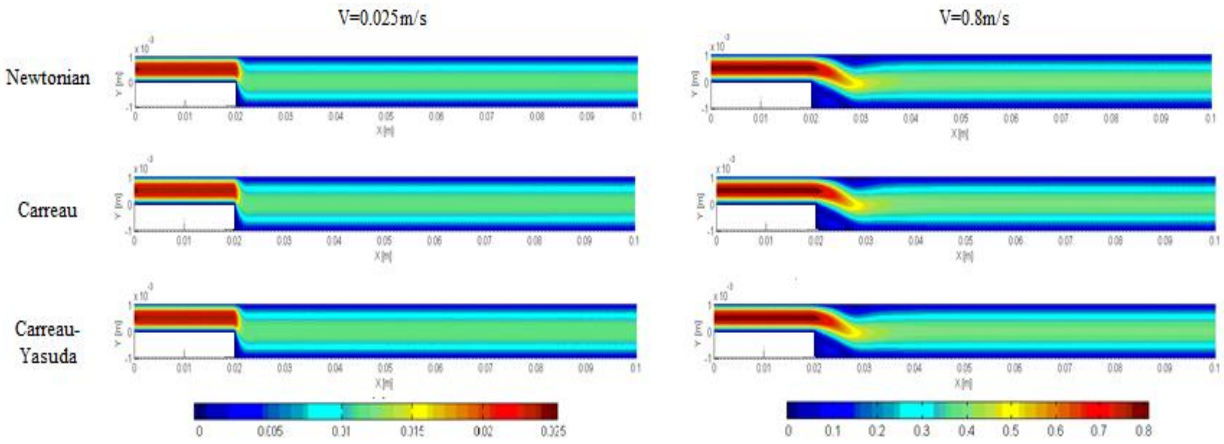

Figure 3. Comparison of velocity profiles between different fluid viscosity models:
Newtonian, Carreau and Carreau-Yasuda

5.2 Topology Optimization of Bidimensional Channel

The topology optimization has been implemented to find the optimal geometry between two inlets and two outlets, as represented in Fig.4. The initial domain is composed of pure fluid material (ρ = 0). The following boundary conditions are applied: parabolic velocity profile, with maximum velocity at the center Vmax = 0.1 m/s, in the inlets and outlets and no-split condition (V = 0) in the walls. Also, the volume constraint limits the total amount of fluid to 50% of the domain.

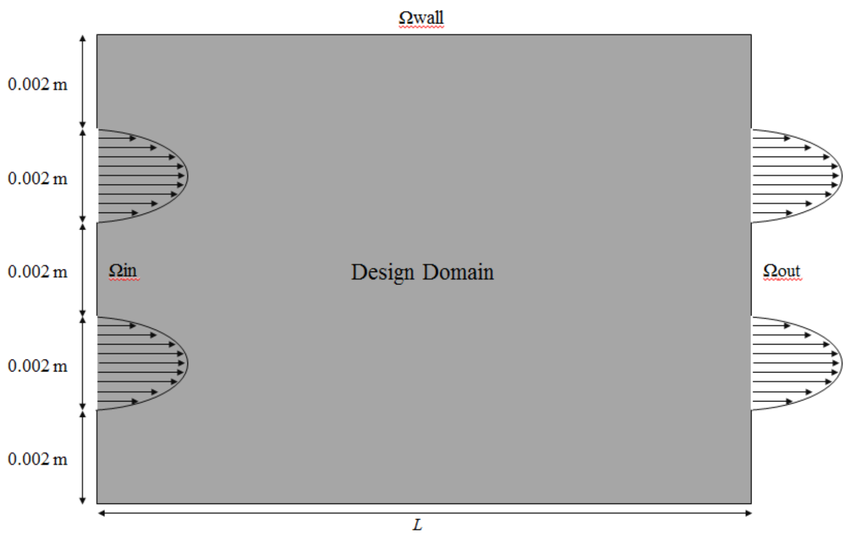

Figure 4. System dimensions and configuration for channel topology optimization.

As shown in previous works, the geometry obtained by the topology optimization method varies according to the length L (BORRVALL e PETERSON, 2003), as this dimension increases the two channels connecting the outlets to the inlets tend to get closer and become one. Is it shown in Fig. 5, three distinct topologies obtained for different values of L. The fluid domain is represented by red path whereas the solid domain is represented by blue path.

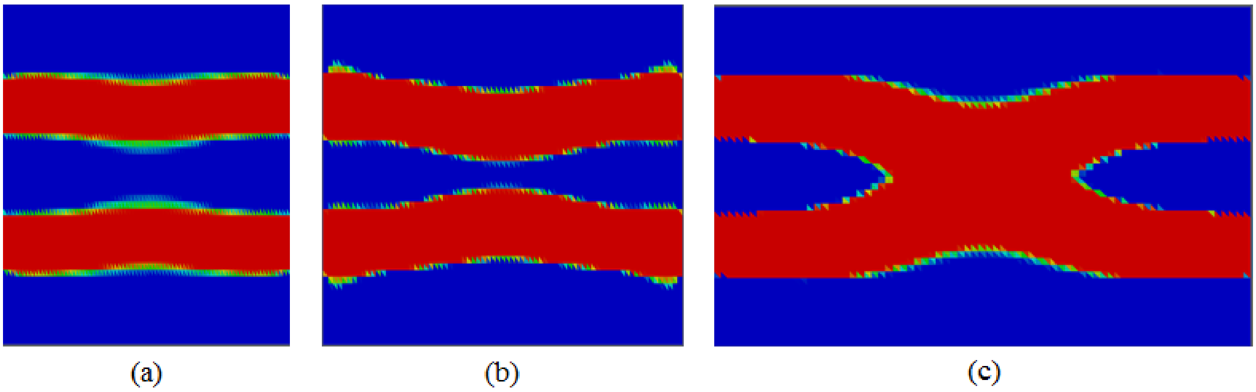

Figure 5. Different topologies obtained with variation of the length L.
(a) L = 0.008m, (b) L =0. 01m, (c) (b) L =0. 015m.

Table 1 shows comparative values obtained for this three topologies: the percentage of volume occupied by fluid in relation to the total volume of the domain, and the value of the optimized functional, defined as in section 3.2.

Table 1. Comparative values of optimization results.

Length L (m)	Volume (%)	Functional Value
0.008	49.75	$5.01 \cdot 10^{-6}$
0.01	49.77	$5.87 \cdot 10^{-6}$
0.015	49.88	$5.92 \cdot 10^{-6}$

The velocity field and the dynamic viscosity distribution for the optimal design obtained for L = 0.015m are shown in Fig. 6.

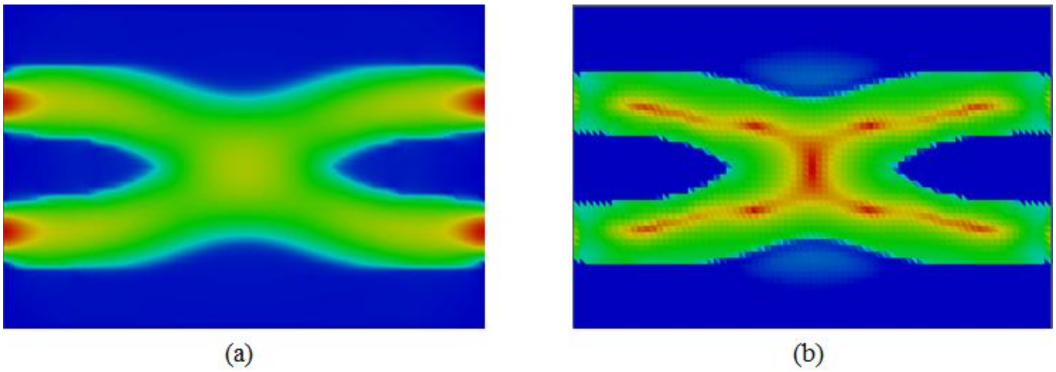

Figure 6. Optimized topology of bidimensional channel for L =0.015m.
(a) Velocity Field, (b) Dynamic Viscosity.

6. CONCLUSIONS

A methodology for design channel for non-Newtonian fluid flow based on topology optimization is presented. Carreau-Yasuda shear thinning model is coupled with the Navier-Stokes equations to represent the more accurately non-Newtonian effects in blood. In topology optimization for Newtonian fluids, a porous material model is used to allow a continuous transition between fluid and solid, where the inverse permeability α is interpolated as a function of the design variable ρ. In order to avoid numerical instabilities when applying the topology optimization method for non-

Newtonian fluids, this material model is adapted by adding an interpolation function of the dynamic viscosity μ, which is also dependent of the pseudo-density ρ.

The results show that the numerical formulation adopted is consistent with the literature, obtaining non-intuitive solutions that minimize the fluidic system dissipation of energy and respect the volume constraint imposed. It is also shown that the FEniCS software platform is a valid tool to automate the finite element method and optimization algorithm, simplifying the coding and implementation of topology optimization problems.

As future work, it intended to investigate more complex models, including body forces, and different geometries and boundary conditions and multi-objective functions, that minimize both energy dissipation and wall shear stress.

7. ACKNOWLEDGEMENTS

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