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**An ALE-FE Method for Vorticity-Streamfunction
Formulation with Species Transport Equation**

Rio de Janeiro, Brazil

2020

Leandro Marques dos Santos

An ALE-FE Method for Vorticity-Streamfunction Formulation with Species Transport Equation



Master's Thesis presented to the Mechanical Engineering Graduate Program of State University of Rio de Janeiro (UERJ) as a pratial requirement to obtain the degree of Master in Sciences. Field of concentration: Transport Phenomena.

Advisor: Prof. Gustavo Rabello dos Anjos, Ph.D.
Co-Advisor: Prof. José da Rocha Miranda Pontes, D.Sc.

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ABSTRACT

Marques, Leandro *An ALE-FE Method for Vorticity-Streamfunction Formulation with Species Transport Equation.* xxf. Master's Thesis (Master of Mechanical Engineering) - Engineering Departament, State University of Rio de Janeiro (UERJ), Rio de Janeiro, Brazil, 2020.

The present work aims at developing a computational framework to simulate blood flow in coronary artery with drug-eluting stent placed using Vorticity-Streamfunction Formulation in an Arbitrary Lagrangian-Eulerian (ALE) approach. The blood was modeled as single-phase, incompressible and newtonian fluid and. The Navier-Stokes equation is shown according to the vorticity-streamfunction formulation with pecies transport equation. The Finite Element Method (FEM) is used to solve the governing equations where the Galerkin formulation was used to discretized the equations in space and the semi-Lagrangian method was used to discretized the material derivative using first order backward difference scheme. The linear systems was solved using Conjugate Gradient Iterative Method.

Keywords: Abritary Lagrangian-Eulerian; Vorticity-Streamfunction Formulation; Finite Element Method; semi-Lagrangian Method; Drug-Eluting Stent.

RESUMO

Marques, Leandro *Um Método FE-ALE para a Formulação Corrente-Vorticidade com a Equação de Transporte de Espécie Química.* xx. Dissertação de Mestrado (Mestrado em Engenharia Mecânica) - Faculdade de Engenharia, Universidade do Estado do Rio de Janeiro (UERJ), Rio de Janeiro, Brasil, 2020.

O presente trabalho tem como objetivo o desenvolvimento de uma estrutura computacional para simular o escoamento sanguíneo em uma artéria coronária com stent farmacológico implantado usando a Formulação Corrente-Vorticidade em uma abordagem Lagrangeana-Euleriana Arbitrária (ALE). O sangue foi modelado como um fluido monofásico, incompressível e newtoniano. A equação de Navier-Stokes é apresentada segundo a formulação corrente-vorticidade com a equação de transporte de espécie química. O Método dos Elementos Finitos (FEM) é usado para resolver as equações de governo, onde a formulação de Galerkin foi usada para discretização no espaço, enquanto o Método semi-Lagrangeano foi usado para discretizar a derivada material usando o *backward difference scheme*. Os sistemas lineares foram resolvidos utilizando o Método Iterativo Gradientes Conjugados.

Palavras-chave: Lagrangeana-Euleriana Arbitrária; Formulação Corrente-Vorticidade; Método dos Elementos Finitos; Método semi-Lagrangeano; Stent Farmacológico.

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INTRODUCTION

According to the World Health Organization (WHO), more people die each year from cardiovascular disease (CVD) than any other cause in the world every year [3]. It is estimated that 17.7 million people died from CVD in 2015, representing 31% of all deaths in the world. About 40% of CVD deaths occurred due to coronary artery disease (CAD). The main cause of CAD is the atherosclerosis which consists of the accumulation of fatty plaques inside the artery wall causing a decrease in lumen diameter. The Atherosclerosis can be prevented with a change in harmful habits such as: cigarette smoking, physical inactivity/low fitness and poor dietary habits [4]. For a corrective approach, however, two treatments can be performed: the *Coronary Artery Bypass Sugery* (CABG) and *Percutaneous Transluminal Coronary Angioplasty* (PTCA). The PTCA a procedure minimally invasive where a wire tube, called *stents* is placed [?]. The main objectives of this work plan are the development of a Finite Element code using the Lagragian-Eulerian Arbitrary (ALE) description for the linear momentum conservation and for species transport equationin an incompressible, one-phase and newtonian fluid, in addtion to know the dynamics of blood flow in a coronary artery with atherosclerosis and drug-eluting stent placed.

The equations that govern the dynamics of blood flow in a coronary artery were developed according to the continuum hypothesis. In this way, the principles of mass conservation, linear momentum conservation and chemical species were used. The blood was considered as an incompressible, newtonian and one-phase fluid, as well as the diffusive coefficient was approximated as constante. The Navier-Stokes equation is shown according to the vorticity-streamfunction formulation with species transport equation without internal source term.

The domain were discretized over an unstructured triangular mesh generated by GMSH open source [42] and the Finite Element Method (FEM) were used. Due to decoupling between the velocity and pressure fields provided by vorticity-streamfunction formulation, the linear triangular element can be used without breaking the Babuska-Brezzi restriction [39] [40]. The Navier-Stokes and Species Transport equations were discretized in time using the Taylor series and the semi-Lagragian Methodo [?] was used in order to reduce spurious oscillations that are usually seen in the diffusion-convection equations. Finally, Galerkin Method was used to discretize the equations in space.

The computational development was done in Python [41] using Object-Oriented Paradigm (OOP) and the Chapter 4 presents the simulation process scripts in addition to the solution algorithm. The numerical code validation was performed by comparison between numerical and analytical solutions in three benchmark problems: *Couette Flow*, *Poiseuille Flow* and *Half Poiseuille Flow*. The horizontal and vertical velocities in *Lid-Driven Cavity* was compared with those presented by *Ghia et al.* [7] and *Marchi et al.* [8]. Then, the comparison of the Taylor-Galerkin and semi-Lagrangian Methods is presented when spurious oscillations are present in a pure convective flow.

The blood flow hydrodynamics and the species chemical transport in coronary artery were simulated in 4 geometries types as suggested by *Wang et al.* [9], but with some modifications to the cartesian coordinates. These geometries types consist of one: (1) coronary artery with atherosclerosis with 40% lumen obstruction; (2) coronary artery with atherosclerosis and with drug-eluting stent placed; (3) real coronary artery with atherosclerosis with 40% lumen obstruction; (4) real coronary artery with atherosclerosis and with drug-eluting stent placed. The numerical simulation visualization was performed using *Paraview* open source as proposed by *Henderson (2007)* [10].

This work was organized as follows:

- Introduction
- Chapter 1: Literature Review
- Chapter 2: Governing Equations
- Chapter 3: Finite Element Method
- Chapter 4: Numerical Code
- Chapter 5: Validation
- Chapter 6: Results
- Conclusion

1 LITERATURE REVIEW

1.1 Introduction

In this chapter, the literature review is presented and discussed, addressing the problem and the methodology used in this work, such as the drug-eluting stents and the Finite Element Method applied to the convection-diffusion equation.

1.2 Drug-Eluting Stent

According to the World Health Organization (WHO) [?], cardiovascular diseases are the main causes of death in the world. About 40% of these deaths are caused by coronary artery disease (CAD).

In 1964, Dotter and Judkins [11] introduced a new technique for obstructed femoral artery treatment due to atherosclerosis. This technique is known as *percutaneous transluminal angioplasty* and it consists of a simple and minimally invasive procedure, allowing execution by any doctor familiar with a vascular catheterization. Such procedure is presented applicable to other arteries, including the coronary artery.

In 1979, Gruntzig, Senning and Seigenthaler [12] performed the percutaneous transluminal technique in the artery coronary artery using a balloon catheter in order to dilate the site with stenosis. The procedure was performed on 50 patients for 18 months and satisfactory results were presented, mainly with patients with only a single artery with stenosis. Such procedure is known as *Coronary Angioplasty Percutaneous Transluminal* (PTCA).

Although PTCA using a balloon has shown satisfactory results, over time, the artery presented restenosis. In 1987, Sigwart et al. [13] present the result of implanting a prosthesis made of a self-expanding stainless steel mesh in the femoral and coronary arteries of 25 patients who cases of restenosis. The prosthesis proved to be a interesting way to solve restenosis. This prosthesis was called *stent*.

In 1994, Serruys et al. [14] present a comparison between PTCA procedures using an balloon and stent implantation. 520 patients were analyzed, where 262 patients with implanted stents and 258 patients with the inflatable balloon. The clinical and angiographic results were better for the patients who had stent implantation to those who underwent the

procedure only using the balloon. Thus, the PTCA procedure with stent implantation was confirmed as a more effective solution than PTCA using only the balloon. However, a problem persisted: the restenosis. During the 1990s, researchers sought to solve this problem. The ?? presents the comparison between PTCA procedures using the balloon and stent.

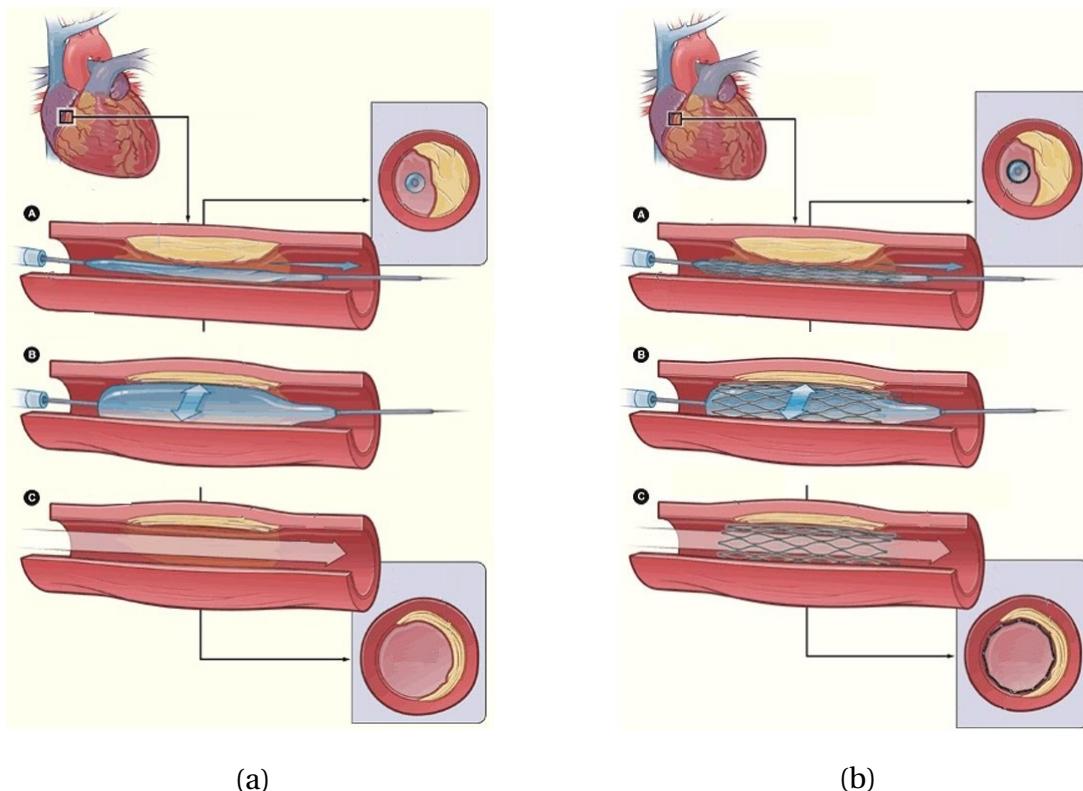


Figure 1: Comparison PTCA procedure: (a) balloon and (b) stent.

In 2001, Hwang, Wu and Edelman [15] presented a simulation of stent implantation coated with a drug in a coronary artery. The simulation presented the close relationship between drug distribution and *Peclet number* in addition to the importance of developing geometries for stents that enhance the diffusion of the chemical substance. Such procedure proved to be a promising option for the treatment of atherosclerosis and reestonosis. This new type of stent would be known as *drug-eluting stent*.

In 2014, Bozsak, Chomaz and Barakat [16] propose a computational model of transport of the drugs *paclitaxel* and *sirolimus* on the artery wall. Such drugs are frequently used in drug-eluting stents. The model takes into account the structure in multilayer of the artery wall and these layers were modeled as porous media. Thus, the law of *Darcy* was used to simulate the flow within the layers of the artery. The simulation showed that the choice of

the type of drug used is a crucial parameter in the creation of the drug-eluting stent due to transport in the artery wall.

Recently, Lucena et al. [17] present the simulation of the transport of the drug *sirolimus* on the wall of an artery modeled as a porous and anisotropic medium. Dissolution in the polymeric stent lining in addition to transport in the artery wall in an axysymmetric domain was considered. The government equations were approximated according to the Finite Element Method. The work showed that the evolution time of the transport process can be efficiently controlled by the diffusion coefficient of the polymer. It is estimated that about 47% of the drug is diffused in the lumen and is lost in the bloodstream. The spatial distribution of the drug, however, is greatly influenced by blood flow and the properties of the artery wall. Thus, such results are susceptible to the patient's health conditions.

In the same year, Wang et al. [9] present the simulation of blood flow in a coronary artery with atherosclerosis and drug-eluting stent placed. Blood is approximated as a Newtonian and monophase fluid and the governing equations were approximated according to the Finite Element Method. Several axisymmetric geometries were presented, including a real coronary artery. Such geometries were used for this current work, but modified for a two-dimensional approach. The simulations showed that the proposed simplified artery with atherosclerosis model produced similar results of velocity, pressure and concentration when compared to the real artery.

Over the past and current decade, several drug-eluting stents have been developed such as: *Ravel* [18], *Taxus I and Taxus II* [19] [20], *C-Sirius* [21], *Smart* [22] and more recent ones as presented in Figure 2. Currently, a new generation of stents has been developed in which the entire structure is absorbed. Such a generation is known as *bioabsorbable stent*, the use of this technology is not the subject of this work.

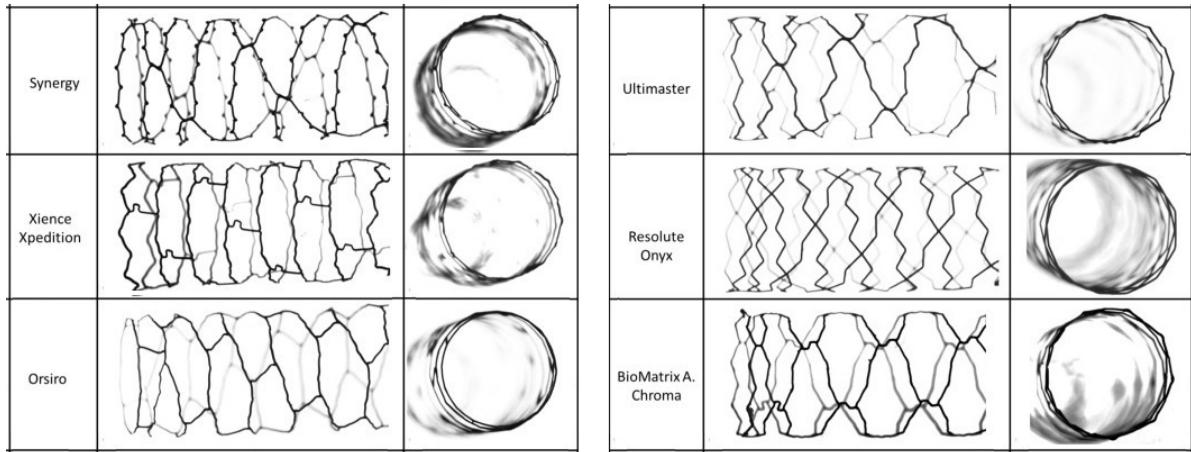


Figure 2: Several models of drug-eluting stent [1].

1.3 Finite Element Method - Convection-Diffusion Equation

The mathematical basis for the Finite Element Method begins in 1909 with Ritz in which a continuous problem is replaced by a discrete problem with a finite number of degrees of freedom where the unknowns were approximated by the product between the constants to be determined and the base functions chosen in order to guarantee the accuracy of the result. This procedure is known as *variational formulation*. Years later, Galerkin uses the Weighted Residual Method to determine the constants of the variational formulation where the same base functions were used in the weight functions. This procedure is known as *Galerkin's formulation* and is widely used nowadays.

During the 1940s, Courant (1943) [23] applied variational formulation to a domain discretized by triangular elements. In 1965, Zienkiewicz and Cheung [24] show that the Weighted Residual Method has a good approximation of the solution and the Finite Element Method was formalized to solve several problems. The proposed mathematical approach is often used today.

The Finite Element Method has become a very effective tool in the solution of several problems and it has been widely used in problems of the solids mechanics. In fluid mechanics, however, its use became possible only later due to the spurious oscillations that it can be seen when the convective term is superior to the diffusive term. Such oscillations are present not only in the Finite Element Method but were also observed in the Finite Difference Method by Spalding in 1972 [25] where it is shown that the *upwind* effect helped to reduce these

oscillations.

In 1976, Christie et al. [26] modify weight functions for asymmetric or quadratic functions to reduce spurious oscillations in one-dimensional diffusion-convection problems. Such modifications produced a *upwind* effect on the solution. This procedure became known as *Petrov Galerkin Formulation*. In the following year, Heinrich, Huyakorn and Zienkiewicz [27] generalize the scheme to a two-dimensional problem. The global matrices, however, became asymmetrical differently from those presented in the Galerkin scheme.

In 1982, Brooks and Hughes [28] proposed a new formulation that consists of modifying the weight functions so that the diffusion operator acts only in the flow direction. This procedure appears in order to eliminate the excess of diffusion perpendicular to the flow that the Petrov-Galerkin scheme presented in some cases. The formulation does not require the use of high-order weight functions and was efficient in eliminating perpendicular diffusion. The formulation received the name *Streamline Upwind Petrov-Galerkin* (SUPG).

In the same year, Pironneau [29] presented the Characteristic Curves Method applied to the Finite Element Method in solving the non-steady convection-diffusion and Navier-Stokes equations. Thereby, the author was able to derive conservative schemes of the type *upwind* with first and second order accurate. As the matrices are symmetric, this scheme proved to be advantageous in solving linear systems compared to other *upwind* schemes. Numerical implementation, however, requires numerical integration in the assembly of the vectors on the right side of the equation. This scheme initiates several works and is known later on as *Characteristic Galerkin*.

In 1984, Donea [5] presents an alternative for solving multidimensional and transient convection-diffusion problems. This alternative is known as the *Taylor-Galerkin* scheme. The scheme consists of using the high-order terms of the Taylor expansion to reduce spurious oscillations. Unlike upwind schemes, in the Taylor-Galerkin scheme there is no need to use modified weight functions. The scheme is compared with the formulations of Galerkin and Petrov Galerkin and showed high precision and low numerical diffusion. Although the Taylor Galerkin and Characteristic Galerkin discretization procedures are distinct, the system of equations is identical for the convection-diffusion equation, where the unknowns is a scalar as mentioned by Lohner [30].

Several researchers have analyzed the stability and convergencei of these schemes

and even the implementation of more efficient schemes has emerged, such as the numerical simulation presented by Anjos et al. in 2006 [31], in which the *semi-Lagrangian* scheme is implemented in the modeling of flows coupled to the transport of chemical species in a Finite Element approach. This scheme was widely used in meteorology and consists of calculating the material derivative along the characteristic trajectory. The discretization in time is done by first order backward differences while the discretization in space is performed according to the Galerkin scheme. The results showed that the semi-Lagrangian scheme is stable, showing no spurious oscillations and excessive numerical diffusion even for long time steps and high Reynolds and Schmidt numbers. Spurious oscillations in the Galerkin, SUPG and semi-Lagrangian schemes are compared by Silva (2011) [2] and they are presented in ??.

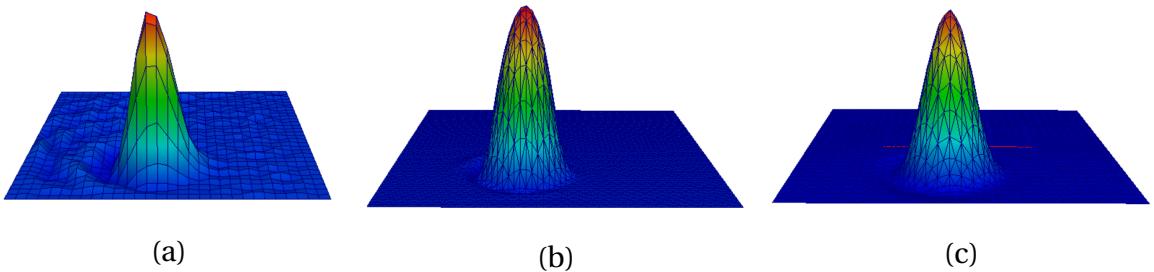


Figure 3: Comparison between spurious oscillations [2]: (a) Galerkin, (b) SUPG e (c) semi-Lagrangian.

The scheme choice to be used to reduce spurious oscillations is related to its advantages and disadvantages when compared to other schemes. In comparison to the Petrov-Galerkin and SUPG schemes, the Taylor-Galerkin, Characteristic and semi-Lagrangian schemes have the advantage of generating symmetric matrices facilitating computational implementation. Whereas, although the effectiveness of the semi-Lagrangian scheme is well known, it requires an efficient search algorithm for neighboring nodes to perform the interpolation. However, in Taylor-Galerkin and Characteristic Galerkin schemes, this need does not exist, so computational implementation becomes smooth. In addition, the system of linear equations generated by the Taylor-Galerkin scheme is similar to that generated by the Characteristic Galerkin scheme when the unknowns are scalar. Thus, the choice between these two schemes does not matter because they produce similar results although the discretization process is different.

All the schemes presented have satisfactory results and they are well known in the literature. These schemes, therefore, made it possible to solve convective problems using

the Finite Element Method. In this work, the semi-Lagragina scheme was chosen for the simulations.

2 GOVERNING EQUATIONS

2.1 Introduction

In this work, the fluid is considered as a continuum medium. This means that given an element of infinitesimal fluid, it is large enough that there are no empty spaces in its domain. Thereby, the flow can be modeled according to universal conservation principles such as:

- Mass Conservation
- Linear Momentum Conservation
- Species Transport Conservation

These are the principles that govern the flow proposed in this work. In the section 2.2, we will present the principle of mass conservation and the *continuity equation* for an incompressible fluid. In the section 2.3, the *Navier Stokes equation* for an incompressible fluid is presented according to the principle of momentum linear conservation for a fluid element. In the section 2.4, we will present the *Species Transport Conservation*. Then, the governing equations are non-dimensionalization in the 2.5 section and the Navier-Stokes equation is presented according to *vorticity-streamfunction formulation* in the 2.6 section.

2.2 Mass Conservation

As presented by Pontes and Mangiavacchi (2016) [32], the principle of mass conservation without source term establishes that:

$$\left[\begin{array}{l} \text{Mass accumulation rate} \\ \text{on control volume} \end{array} \right] = - \left[\begin{array}{l} \text{Mass flux crossing} \\ \text{the boundary} \end{array} \right]$$

Mathematically, the mass accumulation rate within on volume can be represented by:

$$\int_V \frac{\partial}{\partial t} dm \quad (2.1)$$

where the infinitesimal mass dm is defined as $dm = \rho dV$. Replacing it in Eq. 2.1 and considering that the control volume does not vary over time, we have:

$$\int_V \frac{\partial}{\partial t} dm = \int_V \frac{\partial}{\partial t} (\rho dV) = \int_V \frac{\partial \rho}{\partial t} dV + \int_V \rho \frac{\partial dV}{\partial t} = \int_V \frac{\partial \rho}{\partial t} dV \quad (2.2)$$

The mass flux crossing boundary can be mathematically represented by:

$$\oint_S \rho \mathbf{v} \cdot \mathbf{n} dA \quad (2.3)$$

Thereby, according to mass conservation theorem:

$$\int_V \frac{\partial \rho}{\partial t} dV = - \oint_S \rho \mathbf{v} \cdot \mathbf{n} dA \quad (2.4)$$

Applying the *Gauss theorem* on surface integral:

$$\int_V \frac{\partial \rho}{\partial t} dV = - \int_V \nabla \cdot (\rho \mathbf{v}) dV \quad (2.5)$$

that is:

$$\int_V \left[\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right] dV = 0 \quad (2.6)$$

Whereas the $dV \neq 0$, the Eq. 2.6 can be presented as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (2.7)$$

where ρ is density, \mathbf{v} is velocity field whose components are $\mathbf{v} = [u, v]$, ∇ is Del operator whose components are $\nabla = [\partial/\partial x, \partial/\partial y]$, x and y are coordinates components and t is time. The Eq.

2.7 is known as *Continuity Equation*. Developing the equation, we have:

$$\frac{\partial \rho}{\partial t} + \mathbf{v} \cdot \nabla \rho + \rho \nabla \cdot \mathbf{v} = 0 \quad (2.8)$$

According to fluid incompressible assumption, the density does not depend on time and on coordinates. Thereby, the $\partial \rho / \partial t$ e $\nabla \rho$ derivatives are null values. Thus, the mass conservation is reduced to:

$$\rho \nabla \cdot \mathbf{v} = 0 \quad (2.9)$$

that is:

$$\nabla \cdot \mathbf{v} = 0 \quad (2.10)$$

This equation is the *continuity equation* for an incompressible flow.

2.3 Linear Momentum Conservation

The same concept of mass conservation is applied to the linear momentum conservation. Therefore, the principle of linear momentum conservation establishes that:

$$\begin{bmatrix} \text{Linear momentum} \\ \text{accumulation rate} \\ \text{on control volume} \end{bmatrix} = - \begin{bmatrix} \text{Linear momentum} \\ \text{flux crossing} \\ \text{the boundary} \end{bmatrix} + \begin{bmatrix} \text{The resultant of} \\ \text{body force and} \\ \text{surface force} \end{bmatrix}$$

Mathematically, linear momentum accumulation rate on control volume can be presented to represented by:

$$\int_V \frac{\partial}{\partial t} (\rho \mathbf{v}) dV \quad (2.11)$$

The linear momentum flux crossing the boundary can be represented mathematically by:

$$\oint_S \rho \mathbf{v} \cdot \mathbf{n} dA \quad (2.12)$$

The resultant force is consists of surface force and body force. The surface force can be represented by:

$$\oint_S \sigma \cdot \mathbf{n} dA \quad (2.13)$$

where σ is the stress tensor. Whereas, the body is represend by:

$$\int_V \rho \mathbf{g} dV \quad (2.14)$$

where \mathbf{g} is gravity vector. Thereby, according to principle of linear momentum conservation:

$$\int_V \frac{\partial}{\partial t}(\rho \mathbf{v}) dV = - \oint_S \rho \mathbf{v} \cdot \mathbf{n} dA + \oint_S \sigma \cdot \mathbf{n} dA + \int_V \rho \mathbf{g} dV \quad (2.15)$$

Applying the *Gauss Theorem* on surface integrals:

$$\int_V \frac{\partial}{\partial t}(\rho \mathbf{v}) dV = - \int_V \nabla \cdot (\rho \mathbf{v}) dV + \int_V \nabla \cdot \sigma dV + \int_V \rho \mathbf{g} dV \quad (2.16)$$

that is:

$$\int_V \left[\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v}) - \nabla \cdot \sigma - \rho \mathbf{g} \right] dV = 0 \quad (2.17)$$

Whereas the $dV \neq 0$, the Eq. 2.17 can be presented as:

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v}) - \nabla \cdot \sigma - \rho \mathbf{g} = 0 \quad (2.18)$$

that is:

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \nabla \cdot (\rho \mathbf{v}) = \nabla \cdot \sigma + \rho \mathbf{g} \quad (2.19)$$

Developing the left hand side of equation, we have:

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \frac{\partial \rho}{\partial t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} + \mathbf{v} \cdot \nabla(\rho \mathbf{v}) = \rho \left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] + \mathbf{v} \left[\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{v}) \right] \quad (2.20)$$

The last term of above equation is null because the *continuity equation* (Eq. 2.7). Thus, the linear momentum equation can be rewritten as:

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] = \nabla \cdot \boldsymbol{\sigma} + \rho \mathbf{g} \quad (2.21)$$

The stress tensor $\boldsymbol{\sigma}$ can be split into two tensors:

$$\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\tau} \quad (2.22)$$

where, p is pressure field, \mathbf{I} is the identity matrix and $\boldsymbol{\tau}$ is deviatoric stress. Replacing them in Eq. 2.21, we have:

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] = \nabla \cdot [-p\mathbf{I} + \boldsymbol{\tau}] + \rho \mathbf{g} \quad (2.23)$$

that is:

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] = -\nabla p + \nabla \cdot \boldsymbol{\tau} + \rho \mathbf{g} \quad (2.24)$$

The deviatoric stress $\boldsymbol{\tau}$ depends on strain tensor rate and we can define it relating to medium physical properties. Whereas a homogeneous, isotropic fluid and the deviatoric stress as a continuous and linear function of velocity gradient, we have:

$$\boldsymbol{\tau} = \mu [\nabla \mathbf{v} + (\nabla \mathbf{v})^T] + \lambda \mathbf{I} \nabla \cdot \mathbf{v} \quad (2.25)$$

where μ is dynamic viscosity of fluid, λ is known as the second viscosity coefficient and \mathbf{I} is

identity matrix. Replacing them in Eq. 2.24, we have:

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] = -\nabla p + \nabla \cdot [\mu [\nabla \mathbf{v} + (\nabla \mathbf{v})^T] + \lambda \mathbf{I} \nabla \cdot \mathbf{v}] + \rho \mathbf{g} \quad (2.26)$$

that is:

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] = -\nabla p + \nabla \cdot [\mu [\nabla \mathbf{v} + (\nabla \mathbf{v})^T]] + \nabla \cdot [\lambda \mathbf{I} \nabla \cdot \mathbf{v}] + \rho \mathbf{g} \quad (2.27)$$

Whereas the dynamic viscosity μ does not depends on coordinates, we have:

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] = -\nabla p + \mu [\nabla \cdot \nabla \mathbf{v} + \nabla \cdot (\nabla \mathbf{v})^T] + \nabla \cdot [\lambda \mathbf{I} \nabla \cdot \mathbf{v}] + \rho \mathbf{g} \quad (2.28)$$

that is:

$$\rho \left[\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right] = -\nabla p + \mu [\nabla^2 \mathbf{v} + \nabla (\nabla \cdot \mathbf{v})] + \nabla \cdot [\lambda \mathbf{I} \nabla \cdot \mathbf{v}] + \rho \mathbf{g} \quad (2.29)$$

According to Eq. 2.10, we have:

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \mathbf{v} + \mathbf{g} \quad (2.30)$$

where ν is the kinematic viscosity of fluid. The Eq. 2.30 is known as *Navier-Stokes Equation* and is valid for a homogeneous, isotropic, incompressible fluid and with viscosity that it does not depends on coordinates.

2.4 Species Transport Conservation

The species transport conservation establish that:

$$\begin{bmatrix} \text{Chemical species} \\ \text{accumulation rate} \\ \text{on control volume} \end{bmatrix} = - \begin{bmatrix} \text{Chemical species} \\ \text{flux crossing} \\ \text{the boundary} \end{bmatrix} + \begin{bmatrix} \text{The resultant of} \\ \text{chemical species} \\ \text{source rate} \end{bmatrix}$$

Mathematically, chemical species accumulation on control volume can be represented by:

$$\int_V \frac{\partial c}{\partial t} dV \quad (2.31)$$

The chemical species flux crossing the boundary can be splitted into two flux:

$$\oint_S c \mathbf{v} \cdot \mathbf{n} dA - \oint_S D \nabla c \cdot \mathbf{n} dA \quad (2.32)$$

where D is coefficient of chemical species diffusion. The resultant of chemical species source rate on volume can be represented by:

$$\int_V \dot{R} dV \quad (2.33)$$

Thereby, according to species transport conservation:

$$\int_V \frac{\partial c}{\partial t} dV = - \oint_S c \mathbf{v} \cdot \mathbf{n} dA + \oint_S D \nabla c \cdot \mathbf{n} dA + \int_V \dot{R} dV \quad (2.34)$$

Applying the *Gauss Theorem* on surface integrals:

$$\int_V \frac{\partial c}{\partial t} dV = - \int_V \nabla \cdot (c \mathbf{v}) dV + \int_V \nabla \cdot (D \nabla c) dV + \int_V \dot{R} dV \quad (2.35)$$

that is:

$$\int_V \left[\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{v}) - \nabla \cdot (D\nabla c) - \dot{R} \right] dV = 0 \quad (2.36)$$

Whereas the $dV \neq 0$, the Eq. 2.36 can be represented by:

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{v}) - \nabla \cdot (D\nabla c) - \dot{R} = 0 \quad (2.37)$$

that is:

$$\frac{\partial c}{\partial t} + \nabla \cdot (c\mathbf{v}) = \nabla \cdot (D\nabla c) + \dot{R} \quad (2.38)$$

Developing the left hand side of equation, we have:

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c + c \nabla \cdot \mathbf{v} = \nabla \cdot (D\nabla c) + \dot{R} \quad (2.39)$$

The last term of above equation is null because the fluid incompressibility assumption (Eq. 2.10), thus:

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \nabla \cdot (D\nabla c) + \dot{R} \quad (2.40)$$

Considering the diffusion coefficient is constant and without chemical species generation, the species transport equation can rewritten as:

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = D \nabla^2 c \quad (2.41)$$

The Eq. 2.41 is known as *Species Transport Equation* for an incompressible fluid, with constant diffusion coefficient and without chemical species generation.

2.5 Non-dimensionalization

In this section, the non-dimensional form of continuity, Navier-Stokes and species transport equations are shown. The non-dimensionalization helps to understand which terms of the equation influence most during a given simulation in addition to allowing experiments with small scale models. The following parameters was used in non-dimensionalization:

$$\begin{aligned} p &= \rho_0 U^2 p^* & c &= (c_s - c_0)c^* + c_0 & v &= v_0 v^* & D &= D_0 D^* & x &= Lx^* \\ \mathbf{v} &= U \mathbf{v}^* & \mathbf{g} &= g_0 \mathbf{g}^* & \rho &= \rho_0 \rho^* & \nabla &= \frac{1}{L} \nabla^* & t &= \frac{L}{U} t^* \end{aligned}$$

where the asterisk identify the non-dimensional unknowns. Replacing the above parameters in Eq. 2.10, we have:

$$\frac{U}{L} \nabla^* \cdot \mathbf{v}^* = 0 \quad (2.42)$$

Multiplying both sides by U/L :

$$\nabla^* \cdot \mathbf{v}^* = 0 \quad (2.43)$$

A similar procedure is performed in Eq. 2.30, that is:

$$\frac{U^2}{L} \frac{\partial \mathbf{v}^*}{\partial t^*} + \frac{U^2}{L} \mathbf{v}^* \cdot \nabla^* \mathbf{v}^* = -\frac{U^2}{L} \frac{1}{\rho^*} \nabla^* p^* + \frac{\nu_0 U}{L^2} \nu^* \nabla^{*2} \mathbf{v}^* + g_0 \mathbf{g}^* \quad (2.44)$$

Multiplying both sides by L/U^2 :

$$\frac{\partial \mathbf{v}^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla^* \mathbf{v}^* = -\frac{1}{\rho^*} \nabla^* p^* + \frac{\nu_0}{UL} \nu^* \nabla^{*2} \mathbf{v}^* + \frac{g_0 L}{U^2} \mathbf{g}^* \quad (2.45)$$

that is:

$$\frac{\partial \mathbf{v}^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla^* \mathbf{v}^* = -\nabla^* p^* + \frac{\nu_0}{UL} \nabla^{*2} \mathbf{v}^* + \frac{g_0 L}{U^2} \mathbf{g}^* \quad (2.46)$$

In the Eq. 2.41, a similar procedure is performed:

$$(c_s - c_0) \frac{U}{L} \frac{\partial c^*}{\partial t^*} + (c_s - c_0) \frac{U}{L} \mathbf{v}^* \cdot \nabla^* c^* = (c_s - c_0) \frac{D_0}{L^2} D^* \nabla^{*2} c^* \quad (2.47)$$

Multiplying both sides by $L/U(c_s - c_0)$, we have:

$$\frac{\partial c^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla^* c^* = \frac{D_0}{UL} D^* \nabla^{*2} c^* \quad (2.48)$$

that is

$$\frac{\partial c^*}{\partial t^*} + \mathbf{v}^* \cdot \nabla^* c^* = \frac{D_0}{UL} \nabla^{*2} c^* \quad (2.49)$$

Important non-dimensional groups are found in Eqs. 2.43, 2.46 and 2.49. The description of these groups are shown below:

- **Reynolds Number (Re):** Is ratio of inertial forces to viscous forces that it acts a moving fluid particle. It is represented by:

$$Re = \frac{UL}{\nu_0} \quad (2.50)$$

where, ν_0 , U and L are kinematic viscosity of fluid, the velocity field and characteristic length, respectively. The Reynolds number is often used to define the flow, where $Re < Re_{critical}$ is a laminar flow and $Re > Re_{critical}$ is a turbulent flow [33].

- **Froude number (Fr):** Is ratio of inertial force to gravitational forces Is represented by:

$$Fr = \frac{U}{\sqrt{g_0 L}} \quad (2.51)$$

where, g_0 is the gravitational acceleration.

- **Mass Péclet number (Pe_m):** Is ratio advective transport to diffusion transport Is represented by:

$$Pe_m = \frac{D_0}{UL} \quad (2.52)$$

where, D_0 is diffusion coefficient of chemical species. The Pe_m number is often shown as the product of two other non-dimensional groups: the *Reynolds number* and the *Schmidt number*.

- **Schmidt number (Sc):** Is ratio hydrodynamic boundary layer thickness to chemical species diffusion. Is represented by:

$$Sc = \frac{\nu_0}{D_0} \quad (2.53)$$

Replacing these non-dimensional groups in Eqs. 2.43, 2.46 and 2.49 and removing the asterisk, we have:

$$\nabla \cdot \mathbf{v} = 0 \quad (2.54)$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{v} + \frac{1}{Fr^2} \mathbf{g} \quad (2.55)$$

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \frac{1}{ReSc} \nabla^2 c \quad (2.56)$$

The Eqs. 2.54, 2.55 e 2.56 are, respectively, non-dimensional form of Continuity, Navier-Stokes and Species Transport equations for a newtonian and incompressible flow.

2.6 Vorticity-Streamfunction Formulation

The Navier-Stokes equation has a strong coupling between the pressure field and the velocity field. This coupling makes it difficult to implement this equation computationally. The Decoupling of pressure and velocity fields is possible by using the *Vorticity-Streamfunction Formulation*. For this, we will replace in the equation 2.55 the following vector identity:

$$\mathbf{v} \cdot \nabla \mathbf{v} = \nabla \frac{\nu^2}{2} - \mathbf{v} \times \nabla \times \mathbf{v} \quad (2.57)$$

Therefore:

$$\frac{\partial \mathbf{v}}{\partial t} + \nabla \frac{v^2}{2} - \mathbf{v} \times \nabla \times \mathbf{v} = -\nabla p + \frac{1}{Re} \nabla^2 \mathbf{v} + \frac{1}{Fr^2} \mathbf{g} \quad (2.58)$$

Computing the curl on both sides of the above equation:

$$\nabla \times \frac{\partial \mathbf{v}}{\partial t} + \nabla \times \nabla \frac{v^2}{2} - \nabla \times \mathbf{v} \times \nabla \times \mathbf{v} = -\nabla \times \nabla p + \frac{1}{Re} \nabla \times \nabla^2 \mathbf{v} + \frac{1}{Fr^2} \nabla \times \mathbf{g} \quad (2.59)$$

that is:

$$\frac{\partial}{\partial t} [\nabla \times \mathbf{v}] + \nabla \times \nabla \frac{v^2}{2} - \nabla \times [\mathbf{v} \times \nabla \times \mathbf{v}] = -\nabla \times \nabla p + \frac{1}{Re} \nabla^2 [\nabla \times \mathbf{v}] + \frac{1}{Fr^2} \nabla \times \mathbf{g} \quad (2.60)$$

The terms that contain the gradient operator cancel each other out, since the curl of gradient of a scalar is zero. The last term is also null because the derivatives of a constant, as in the case of \mathbf{g} , are equal to zero. Thus, we have:

$$\frac{\partial}{\partial t} [\nabla \times \mathbf{v}] - \nabla \times [\mathbf{v} \times \nabla \times \mathbf{v}] = \frac{1}{Re} \nabla^2 [\nabla \times \mathbf{v}] \quad (2.61)$$

The vector $\nabla \times \mathbf{v}$ is known as *vorticity* (w). Therby, the equation can be represented by:

$$\frac{\partial w}{\partial t} - \nabla \times [\mathbf{v} \times w] = \frac{1}{Re} \nabla^2 w \quad (2.62)$$

The second term of left side in Eq. 2.62 can be replaced by following vectorial identity:

$$\nabla \times [\mathbf{v} \times w] = -\mathbf{v} \cdot \nabla w + w \cdot \nabla v \quad (2.63)$$

Thus the Eq. 2.62 will be:

$$\frac{\partial w}{\partial t} + \mathbf{v} \cdot \nabla w - w \cdot \nabla \mathbf{v} = \frac{1}{Re} \nabla^2 w \quad (2.64)$$

For two-dimensional flows, as in the case of this work, the vorticity is perpendicular to the velocity vector. Thus, the product $w \cdot \nabla \mathbf{v}$ will be canceled as presented by Pontes and Mangiavacchi (2016) [32]. Therefore:

$$\frac{\partial w}{\partial t} + \mathbf{v} \cdot \nabla w = \frac{1}{Re} \nabla^2 w \quad (2.65)$$

The Eq. 2.65 is known as *vorticity equation* for two-dimensional flows of a Newtonian and incompressible fluid. For a steady and two-dimensional flow of incompressible fluid, the velocity can be calculated from the volumetric flux. Thereby, the velocity is replaced by a scalar. Such a scalar is known as *streamfunction* (ψ). The relationship between the velocity components and the streamfunction is presented by expanding the continuity equation (Eq. 2.10):

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (2.66)$$

The following relationship between the streamfunction and the velocity components can be defined so that Eq. 2.66 is satisfied:

$$u = \frac{\partial \psi}{\partial y} \quad v = -\frac{\partial \psi}{\partial x} \quad (2.67)$$

The relationship between streamfunction and vorticity is shown expanding the $\nabla \times \mathbf{v}$ operation for the two-dimensional case:

$$\nabla \times \mathbf{v} = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y} \quad (2.68)$$

Replacing the Eq. 2.67 in Eq. 2.68, we that:

$$w = -\frac{\partial}{\partial x} \frac{\partial v}{\partial x} - \frac{\partial}{\partial y} \frac{\partial u}{\partial y} \quad (2.69)$$

that is:

$$w = -\nabla^2 \psi \quad (2.70)$$

Therefore, the equations that govern the proposed problem in its non-dimensional form and vorticity-streamfunction formulation are shown below:

$$\frac{\partial w}{\partial t} + \mathbf{v} \cdot \nabla w = \frac{1}{Re} \nabla^2 w \quad (2.71)$$

$$\nabla^2 \psi = -w \quad (2.72)$$

$$\mathbf{v} = \mathbf{D}\psi \quad (2.73)$$

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \frac{1}{ReSc} \nabla^2 c \quad (2.74)$$

where \mathbf{D} is a differential operator whose components are $[\partial/\partial y, -\partial/\partial x]$.

3 FINITE ELEMENT METHOD

3.1 Introduction

In this chapter, we will describe the Finite Element Method (FEM). While the Finite Difference Method (MDF) represents a direct approximation to the differential equations, the proposal of the finite element procedure is an approximation applied to the terms of the variational formulation as mentioned by Zienkiewicz and Cheung (1965) [24]. For more details on the Finite Element Method see the works of Zienkiewicz and Taylor (2000) [6], Hughes (2000) [34] and Fish and Belytschko (2007) [35].

First, we will discretize the governing equations in time using the Taylor series approximation, keeping the second order terms of the expansion in order to reduce the spurious oscillations present in the convection-diffusion equations as in the case of the vorticity and concentration equations. Then, we will present the strong formulation of them. That done, the weak formulation of the governing equations is presented and they are discretized in space using Galerkin's Method with a linear triangular element. Therefore, the government equations in the matrix form according to the *Taylor-Galerkin* Method are presented. For more details on the scheme, see the work of Donea (1984) [5].

3.2 Strong Formulation

Governing equations in differential form with boundary conditions are known as **Strong Formulation**. Thus, the strong formulation for the proposed problem is:

$$\dot{w} + \mathbf{v} \cdot \nabla w = \frac{1}{Re} \nabla^2 w + \frac{\Delta t}{2} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla w] \quad (3.1)$$

$$\nabla^2 \psi = -w \quad (3.2)$$

$$\mathbf{v} = \mathbf{D}\psi \quad (3.3)$$

$$\dot{c} + \mathbf{v} \cdot \nabla c = \frac{1}{ReSc} \nabla^2 c + \frac{\Delta t}{2} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla c] \quad (3.4)$$

These equations are valid in $\Omega \subset \mathbb{R}^2$ domain with the following boundary conditions:

$$\begin{aligned} w &= w_\Gamma \quad \text{in } \Gamma_1 \\ \psi &= \psi_\Gamma \quad \text{in } \Gamma_2 \\ \mathbf{v} &= \mathbf{v}_\Gamma \quad \text{in } \Gamma_3 \\ c &= c_\Gamma \quad \text{in } \Gamma_4 \end{aligned} \tag{3.5}$$

3.3 Weak Formulation

The result of the weighted governing equations over the domain is known as **Weak formulation** as mentioned by Anjos (2007) [36]. Next, we will present the weak formulation for a single-phase, Newtonian and incompressible fluid using the vorticity-streamfunction formulation with species transport equation. For more details, see the work of Brenner and Scott (1994) [37]. As the objective is to find an approximate solution, it is acceptable to assume that a **Residue R** is produced in the governing equations, that is:

$$\dot{w} + \mathbf{v} \cdot \nabla w - \frac{1}{Re} \nabla^2 w - \frac{\Delta t}{2} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla w] = R_1 \tag{3.6}$$

$$\nabla^2 \psi + w = R_2 \tag{3.7}$$

$$\mathbf{v} - \mathbf{D}\psi = R_3 \tag{3.8}$$

$$\dot{c} + \mathbf{v} \cdot \nabla c - \frac{1}{ReSc} \nabla^2 c - \frac{\Delta t}{2} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla c] = R_4 \tag{3.9}$$

We will try to force the residue to be equivalent to zero in a weighted sense as mentioned by Finlayson (1972) [38], then:

$$\int_{\Omega} R_1 \cdot \delta d\Omega = 0 \quad (3.10)$$

$$\int_{\Omega} R_2 \cdot \phi d\Omega = 0 \quad (3.11)$$

$$\int_{\Omega} R_3 \cdot \xi d\Omega = 0 \quad (3.12)$$

$$\int_{\Omega} R_4 \cdot \eta d\Omega = 0 \quad (3.13)$$

where δ, ϕ, ξ e η are weight function. The weight functions are a set of arbitrary functions that belong to a function space that will be discussed later. We then have the following integrals:

$$\int_{\Omega} \left\{ \dot{w} + \mathbf{v} \cdot \nabla w - \frac{1}{Re} \nabla^2 w - \frac{\Delta t}{2} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla w] \right\} \cdot \delta d\Omega = 0 \quad (3.14)$$

$$\int_{\Omega} \{\nabla^2 \psi + w\} \cdot \phi d\Omega = 0 \quad (3.15)$$

$$\int_{\Omega} \{\mathbf{v} - \mathbf{D}\psi\} \cdot \xi d\Omega = 0 \quad (3.16)$$

$$\int_{\Omega} \left\{ \dot{c} + \mathbf{v} \cdot \nabla c - \frac{1}{ReSc} \nabla^2 c - \frac{\Delta t}{2} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla c] \right\} \cdot \eta d\Omega = 0 \quad (3.17)$$

Developing the integrals, we have:

$$\int_{\Omega} \dot{w} \delta d\Omega + \int_{\Omega} \mathbf{v} \cdot \nabla w \delta d\Omega - \frac{1}{Re} \int_{\Omega} \nabla^2 w \delta - \frac{\Delta t}{2} \int_{\Omega} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla w] \delta d\Omega = 0 \quad (3.18)$$

$$\int_{\Omega} \nabla^2 \psi \phi d\Omega + \int_{\Omega} w \phi d\Omega = 0 \quad (3.19)$$

$$\int_{\Omega} \mathbf{v} \cdot \nabla \xi d\Omega - \int_{\Omega} \mathbf{D} \psi \cdot \nabla \xi d\Omega = 0 \quad (3.20)$$

$$\int_{\Omega} \dot{c} \eta d\Omega + \int_{\Omega} \mathbf{v} \cdot \nabla c \eta d\Omega - \frac{1}{ReSc} \int_{\Omega} \nabla^2 c \eta d\Omega - \frac{\Delta t}{2} \int_{\Omega} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla c] \eta d\Omega = 0 \quad (3.21)$$

In the diffusive term of the equations (3.18, 3.19 and 3.21), we will apply Green's theorem in order to decrease the derivative order and separate the term evaluated in the boundary. Thus the diffusive term will become:

$$-\frac{1}{Re} \int_{\Omega} \nabla^2 w \delta d\Omega = \frac{1}{Re} \int_{\Omega} \nabla w \cdot \nabla \delta d\Omega - \frac{1}{Re} \int_{\Gamma} \delta \nabla w \cdot \mathbf{n} d\Gamma \quad (3.22)$$

$$\int_{\Omega} \nabla^2 \psi \phi d\Omega = - \int_{\Omega} \nabla \psi \cdot \nabla \phi d\Omega + \int_{\Gamma} \phi \nabla \psi \cdot \mathbf{n} d\Gamma \quad (3.23)$$

$$-\frac{1}{ReSc} \int_{\Omega} \nabla^2 c \eta d\Omega = \frac{1}{ReSc} \int_{\Omega} \nabla c \cdot \nabla \eta d\Omega - \frac{1}{ReSc} \int_{\Gamma} \eta \nabla c \cdot \mathbf{n} d\Gamma \quad (3.24)$$

where \mathbf{n} is the normal vector oriented outside the Γ . The last term in the above equations is known as a natural condition. As presented in the section 3.2, for the problem proposed in this work, we have only Dirichlet conditions (known as an essential condition).

Therefore, we will consider $\delta = 0$, $\phi = 0$ and $\eta = 0$ assumptions in the equations (3.22, 3.23 and 3.24) for all Γ . Thereby, the integral in Γ will be null and the diffusive term of the equations (3.18, 3.19 and 3.21) become:

$$-\frac{1}{Re} \int_{\Omega} \nabla^2 w \delta d\Omega = \frac{1}{Re} \int_{\Omega} \nabla w \cdot \nabla \delta d\Omega \quad (3.25)$$

$$\int_{\Omega} \nabla^2 \psi \phi d\Omega = - \int_{\Omega} \nabla \psi \cdot \nabla \phi d\Omega \quad (3.26)$$

$$-\frac{1}{ReSc} \int_{\Omega} \nabla^2 c \eta d\Omega = \frac{1}{ReSc} \int_{\Omega} \nabla c \cdot \nabla \eta d\Omega \quad (3.27)$$

For the numerical diffusivity term of the equations (3.18 and 3.21), we will apply a procedure similar to the previous one. Thus, the term of numerical diffusivity will be:

$$-\frac{\Delta t}{2} \int_{\Omega} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla w] \delta d\Omega = \frac{\Delta t}{2} \int_{\Omega} [\mathbf{v} \cdot \nabla w] \mathbf{v} \cdot \nabla \delta d\Omega - \frac{\Delta t}{2} \int_{\Gamma} [\mathbf{v} \cdot \nabla w] \delta \mathbf{v} \cdot \mathbf{n} d\Gamma \quad (3.28)$$

$$-\frac{\Delta t}{2} \int_{\Omega} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla c] \eta d\Omega = \frac{\Delta t}{2} \int_{\Omega} [\mathbf{v} \cdot \nabla c] \mathbf{v} \cdot \nabla \eta d\Omega - \frac{\Delta t}{2} \int_{\Gamma} [\mathbf{v} \cdot \nabla c] \eta \mathbf{v} \cdot \mathbf{n} d\Gamma \quad (3.29)$$

In the same way, we can cancel the natural condition term according to the assumption previously adopted. Therefore, the numeric diffusivity term for the equations (3.18 and 3.21) will be:

$$-\frac{\Delta t}{2} \int_{\Omega} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla w] \delta d\Omega = \frac{\Delta t}{2} \int_{\Omega} [\mathbf{v} \cdot \nabla w] \mathbf{v} \cdot \nabla \delta d\Omega \quad (3.30)$$

$$-\frac{\Delta t}{2} \int_{\Omega} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla c] \eta d\Omega = \frac{\Delta t}{2} \int_{\Omega} [\mathbf{v} \cdot \nabla c] \mathbf{v} \cdot \nabla \eta d\Omega \quad (3.31)$$

Therefore, replacing the new diffusive terms in the governing equations:

$$\int_{\Omega} \dot{w} \delta d\Omega + \int_{\Omega} \mathbf{v} \cdot \nabla w \delta d\Omega + \frac{1}{Re} \int_{\Omega} \nabla w \cdot \nabla \delta d\Omega + \frac{\Delta t}{2} \int_{\Omega} [\mathbf{v} \cdot \nabla w] \mathbf{v} \cdot \nabla \delta d\Omega = 0 \quad (3.32)$$

$$-\int_{\Omega} \nabla \psi \cdot \nabla \phi d\Omega + \int_{\Omega} w \phi d\Omega = 0 \quad (3.33)$$

$$\int_{\Omega} \mathbf{v} \xi d\Omega - \int_{\Omega} \mathbf{D} \psi \xi d\Omega = 0 \quad (3.34)$$

$$\int_{\Omega} \dot{c} \eta d\Omega + \int_{\Omega} \mathbf{v} \cdot \nabla c \eta d\Omega + \frac{1}{ReSc} \int_{\Omega} \nabla c \cdot \nabla \eta d\Omega + \frac{\Delta t}{2} \int_{\Omega} [\mathbf{v} \cdot \nabla c] \mathbf{v} \cdot \nabla \eta d\Omega = 0 \quad (3.35)$$

If we consider that:

$$\begin{aligned}
 m_1(\dot{w}, \delta) &= \int_{\Omega} \dot{w} \delta d\Omega & m_3(\mathbf{v}, \xi) &= \int_{\Omega} \mathbf{v} \cdot \nabla \xi d\Omega \\
 g_1(\mathbf{v}, \delta) &= \int_{\Omega} \mathbf{v} \cdot \nabla w \delta d\Omega & g_3(\psi, \xi) &= \int_{\Omega} \mathbf{D}\psi \cdot \nabla \xi d\Omega \\
 k_1(w, \delta) &= \int_{\Omega} \nabla w \cdot \nabla \delta d\Omega & m_4(\dot{c}, \eta) &= \int_{\Omega} \dot{c} \eta d\Omega \\
 k_{n1}(w, \delta) &= \int_{\Omega} [\mathbf{v} \cdot \nabla w] \mathbf{v} \cdot \nabla \delta d\Omega & g_4(\mathbf{v}, \eta) &= \int_{\Omega} \mathbf{v} \cdot \nabla c \eta d\Omega \\
 k_2(\psi, \phi) &= \int_{\Omega} \nabla \psi \cdot \nabla \phi d\Omega & k_4(c, \eta) &= \int_{\Omega} \nabla c \cdot \nabla \eta d\Omega \\
 m_2(\psi, \phi) &= \int_{\Omega} w \phi d\Omega & k_{n4}(c, \delta) &= \int_{\Omega} [\mathbf{v} \cdot \nabla c] \mathbf{v} \cdot \nabla \eta d\Omega
 \end{aligned} \tag{3.36}$$

the equations, thus, can be shown in the weak form respectively:

$$m_1(\dot{w}, \delta) + g_1(\mathbf{v}, \delta) + \frac{1}{Re} k_1(w, \delta) + \frac{\Delta t}{2} k_{n1}(w, \delta) = 0 \tag{3.37}$$

$$-k_2(\psi, \phi) + m_2(\psi, \phi) = 0 \tag{3.38}$$

$$m_3(\mathbf{v}, \xi) - g_3(\psi, \xi) = 0 \tag{3.39}$$

$$m_4(\dot{c}, \eta) + g_4(\mathbf{v}, \eta) + \frac{1}{ReSc} k_4(c, \eta) + \frac{\Delta t}{2} k_{n4}(c, \eta) = 0 \tag{3.40}$$

Considering the sets of basis functions:

$$\begin{aligned}
 \mathbb{W} &= \{w \in \Omega \rightarrow \mathbb{R}^2 : \int_{\Omega} w^2 d\Omega < \infty; w = w_{\Gamma}\} \\
 \mathbb{P} &= \{\psi \in \Omega \rightarrow \mathbb{R}^2 : \int_{\Omega} \psi^2 d\Omega < \infty; \psi = \psi_{\Gamma}\} \\
 \mathbb{V} &= \{v \in \Omega \rightarrow \mathbb{R}^2 : \int_{\Omega} v^2 d\Omega < \infty; v = v_{\Gamma}\} \\
 \mathbb{C} &= \{c \in \Omega \rightarrow \mathbb{R}^2 : \int_{\Omega} c^2 d\Omega < \infty; c = c_{\Gamma}\}
 \end{aligned} \tag{3.41}$$

and the set of weight functions space:

$$\begin{aligned}\mathbb{D} &= \{\delta \in \Omega \rightarrow \mathbb{R}^2 : \int_{\Omega} \delta^2 d\Omega < \infty; \delta_{\Gamma} = 0\} \\ \mathbb{F} &= \{\phi \in \Omega \rightarrow \mathbb{R}^2 : \int_{\Omega} \phi^2 d\Omega < \infty; \phi_{\Gamma} = 0\} \\ \mathbb{X} &= \{\xi \in \Omega \rightarrow \mathbb{R}^2 : \int_{\Omega} \xi^2 d\Omega < \infty; \xi_{\Gamma} = 0\} \\ \mathbb{N} &= \{\eta \in \Omega \rightarrow \mathbb{R}^2 : \int_{\Omega} \eta^2 d\Omega < \infty; \eta_{\Gamma} = 0\}\end{aligned}\tag{3.42}$$

The weak formulation consists to find the solutions of $w \in \mathbb{W}$, $\psi \in \mathbb{P}$, $v \in \mathbb{V}$ and $c \in \mathbb{C}$ such that:

$$m_1(\dot{w}, \delta) + g_1(\mathbf{v}, \delta) + \frac{1}{Re} k_1(w, \delta) + \frac{\Delta t}{2} k_{n1}(w, \delta) = 0\tag{3.43}$$

$$-k_2(\psi, \phi) + m_2(\psi, \phi) = 0\tag{3.44}$$

$$m_3(\mathbf{v}, \xi) - g_3(\psi, \xi) = 0\tag{3.45}$$

$$m_4(\dot{c}, \eta) + g_4(\mathbf{v}, \eta) + \frac{1}{ReSc} k_4(c, \eta) + \frac{\Delta t}{2} k_{n4}(c, \eta) = 0\tag{3.46}$$

for all $\delta \in \mathbb{D}$, $\phi \in \mathbb{F}$, $\xi \in \mathbb{X}$ and $\eta \in \mathbb{N}$.

3.4 Galerkin Method

As funções peso δ , ϕ , ξ e η são conjuntos de funções arbitrárias e possuem uma infinidade de escolhas. Neste trabalho para discretizarmos o domínio, utilizaremos a formulação de **Galerkin** que consiste em utilizar as mesmas funções de forma para as funções peso e a função interpoladora da variável em questão (w, ψ, \mathbf{v}, c). Assim, as Eqs. 3.32 a 3.35 podem ser apresentadas na forma expandida tais como:

$$\begin{aligned}\int_{\Omega} \dot{w} \delta d\Omega + \int_{\Omega} u \frac{\partial w}{\partial x} \delta d\Omega + \int_{\Omega} v \frac{\partial w}{\partial y} \delta d\Omega + \frac{1}{Re} \int_{\Omega} \left\{ \frac{\partial w}{\partial x} \frac{\partial \delta}{\partial x} + \frac{\partial w}{\partial y} \frac{\partial \delta}{\partial y} \right\} d\Omega \\ + \frac{\Delta t}{2} \int_{\Omega} u \frac{\partial \delta}{\partial x} \left[u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} \right] d\Omega + \frac{\Delta t}{2} \int_{\Omega} v \frac{\partial \delta}{\partial y} \left[u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} \right] d\Omega = 0\end{aligned}\tag{3.47}$$

$$-\int_{\Omega} \left\{ \frac{\partial \psi}{\partial x} \frac{\partial \phi}{\partial x} + \frac{\partial \psi}{\partial y} \frac{\partial \phi}{\partial y} \right\} d\Omega + \int_{\Omega} w \phi d\Omega = 0 \quad (3.48)$$

$$\int_{\Omega} u \xi d\Omega - \int_{\Omega} \frac{\partial \psi}{\partial y} \xi d\Omega = 0 \quad (3.49)$$

$$\int_{\Omega} v \xi d\Omega + \int_{\Omega} \frac{\partial \psi}{\partial x} \xi d\Omega = 0 \quad (3.50)$$

$$\begin{aligned} & \int_{\Omega} c \eta d\Omega + \int_{\Omega} u \frac{\partial c}{\partial x} \eta d\Omega + \int_{\Omega} v \frac{\partial c}{\partial y} \eta d\Omega + \frac{1}{ReSc} \int_{\Omega} \left\{ \frac{\partial c}{\partial x} \frac{\partial \eta}{\partial x} + \frac{\partial c}{\partial y} \frac{\partial \eta}{\partial y} \right\} d\Omega \\ & + \frac{\Delta t}{2} \int_{\Omega} u \frac{\partial \eta}{\partial x} \left[u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} \right] d\Omega + \frac{\Delta t}{2} \int_{\Omega} v \frac{\partial \eta}{\partial y} \left[u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} \right] d\Omega = 0 \end{aligned} \quad (3.51)$$

Discretizaremos, agora, o domínio em ne elementos e np nós, onde ne representa o número total de elementos e np o número total de nós da malha computacional. Desta forma, temos:

$$w(\mathbf{x}, t) \simeq \sum_{i=1}^{np} w_i(t) N_i(\mathbf{x}) \quad (3.52)$$

$$\psi(\mathbf{x}, t) \simeq \sum_{i=1}^{np} \psi_i(t) N_i(\mathbf{x}) \quad (3.53)$$

$$u(\mathbf{x}, t) \simeq \sum_{i=1}^{np} u_i(t) N_i(\mathbf{x}) \quad (3.54)$$

$$v(\mathbf{x}, t) \simeq \sum_{i=1}^{np} v_i(t) N_i(\mathbf{x}) \quad (3.55)$$

$$c(\mathbf{x}, t) \simeq \sum_{i=1}^{np} c_i(t) N_i(\mathbf{x}) \quad (3.56)$$

onde $w_i = [w_1, \dots, w_{np}]$, $\psi_i = [\psi_1, \dots, \psi_{np}]$, $u_i = [u_1, \dots, u_{np}]$, $v_i = [v_1, \dots, v_{np}]$, $c_i = [c_1, \dots, c_{np}]$ são as incógnitas a serem encontradas. Como essas incógnitas dependem apenas do tempo, poderão sair das integrais sobre o domínio Ω e $N_i = [N_1, \dots, N_{np}]$ são as funções de aproxi-

mação conhecidas como funções base ou funções de interpolação. Essas funções podem ser escolhidas de modo arbitrário e devem respeitar as condições de contorno. Elas variam conforme a escolha do tipo de elemento usado na discretização. Conforme foi mencionado, neste trabalho usaremos o mesmo tipo de elemento para cada equação de governo, assim possuiremos as mesmas funções bases para todas as equações.

Na formulação de Galerkin, as funções peso assumem os valores das funções base, isto é:

$$\delta(\mathbf{x}, t) \simeq \sum_{j=1}^{np} \delta_j(t) N_j(\mathbf{x}) \quad (3.57)$$

$$\phi(\mathbf{x}, t) \simeq \sum_{j=1}^{np} \phi_j(t) N_j(\mathbf{x}) \quad (3.58)$$

$$\xi(\mathbf{x}, t) \simeq \sum_{j=1}^{np} \xi_j(t) N_j(\mathbf{x}) \quad (3.59)$$

$$\eta(\mathbf{x}, t) \simeq \sum_{j=1}^{np} \eta_j(t) N_j(\mathbf{x}) \quad (3.60)$$

Desta forma, as equações de governo na forma variacional discretizada no espaço serão:

$$\begin{aligned} & \int_{\Omega} \sum_{i=1}^{np} \dot{w}_i N_i \sum_{j=1}^{np} \delta_j N_j d\Omega + u \int_{\Omega} \sum_{i=1}^{np} \frac{\partial w_i N_i}{\partial x} \sum_{j=1}^{np} \delta_j N_j d\Omega + v \int_{\Omega} \sum_{i=1}^{np} \frac{\partial w_i N_i}{\partial y} \sum_{j=1}^{np} \delta_j N_j d\Omega \\ & + \frac{1}{Re} \int_{\Omega} \left\{ \sum_{i=1}^{np} \frac{\partial w_i N_i}{\partial x} \sum_{j=1}^{np} \frac{\partial \delta_j N_j}{\partial x} + \sum_{i=1}^{np} \frac{\partial w_i N_i}{\partial y} \sum_{j=1}^{np} \frac{\partial \delta_j N_j}{\partial y} \right\} \\ & + \frac{\Delta t}{2} \int_{\Omega} u \sum_{j=1}^{np} \frac{\partial \delta_j N_j}{\partial x} \left[u \sum_{i=1}^{np} \frac{\partial w_i N_i}{\partial x} + v \sum_{i=1}^{np} \frac{\partial w_i N_i}{\partial y} \right] d\Omega \\ & + \frac{\Delta t}{2} \int_{\Omega} v \sum_{j=1}^{np} \frac{\partial \delta_j N_j}{\partial y} \left[u \sum_{i=1}^{np} \frac{\partial w_i N_i}{\partial x} + v \sum_{i=1}^{np} \frac{\partial w_i N_i}{\partial y} \right] d\Omega = 0 \end{aligned} \quad (3.61)$$

$$\begin{aligned} & - \int_{\Omega} \left\{ \sum_{i=1}^{np} \frac{\partial \psi_i N_i}{\partial x} \sum_{j=1}^{np} \frac{\partial \phi_j N_j}{\partial x} + \sum_{i=1}^{np} \frac{\partial \psi_i N_i}{\partial y} \sum_{j=1}^{np} \frac{\partial \phi_j N_j}{\partial y} \right\} d\Omega \\ & + \int_{\Omega} \sum_{i=1}^{np} w_i N_i \sum_{j=1}^{np} \phi_j N_j d\Omega = 0 \end{aligned} \quad (3.62)$$

$$\int_{\Omega} \sum_{i=1}^{np} u_i N_i \sum_{j=1}^{np} \xi_j N_j d\Omega - \int_{\Omega} \sum_{i=1}^{np} \frac{\partial \psi_i N_i}{\partial y} \sum_{j=1}^{np} \xi_j N_j d\Omega = 0 \quad (3.63)$$

$$\int_{\Omega} \sum_{i=1}^{np} v_i N_i \sum_{j=1}^{np} \xi_j N_j d\Omega + \int_{\Omega} \sum_{i=1}^{np} \frac{\partial \psi_i N_i}{\partial x} \sum_{j=1}^{np} \xi_j N_j d\Omega = 0 \quad (3.64)$$

$$\begin{aligned} & \int_{\Omega} \sum_{i=1}^{np} \dot{c}_i N_i \sum_{j=1}^{np} \eta_j N_j d\Omega + u \int_{\Omega} \sum_{i=1}^{np} \frac{\partial c_i N_i}{\partial x} \sum_{j=1}^{np} \eta_j N_j d\Omega + v \int_{\Omega} \sum_{i=1}^{np} \frac{\partial c_i N_i}{\partial y} \sum_{j=1}^{np} \eta_j N_j d\Omega \\ & + \frac{1}{ReSc} \int_{\Omega} \left\{ \sum_{i=1}^{np} \frac{\partial c_i N_i}{\partial x} \sum_{j=1}^{np} \frac{\partial \eta_j N_j}{\partial x} + \sum_{i=1}^{np} \frac{\partial c_i N_i}{\partial y} \sum_{j=1}^{np} \frac{\partial \eta_j N_j}{\partial y} \right\} d\Omega \\ & + \frac{\Delta t}{2} \int_{\Omega} u \sum_{j=1}^{np} \frac{\partial \eta_j N_j}{\partial x} \left[u \sum_{i=1}^{np} \frac{\partial c_i N_i}{\partial x} + v \sum_{i=1}^{np} \frac{\partial c_i N_i}{\partial y} \right] d\Omega \\ & + \frac{\Delta t}{2} \int_{\Omega} v \sum_{j=1}^{np} \frac{\partial \eta_j N_j}{\partial y} \left[u \sum_{i=1}^{np} \frac{\partial c_i N_i}{\partial x} + v \sum_{i=1}^{np} \frac{\partial c_i N_i}{\partial y} \right] d\Omega = 0 \end{aligned} \quad (3.65)$$

Podemos retirar as componentes da velocidade u e v da integral no termo convectivo das equações 3.61 e 3.65 já que as mesmas não serão tratadas como incógnitas, isto é, para a equação da vorticidade usaremos os valores das componentes u e v do passo de tempo anterior enquanto para a equação do transporte de espécie química, as componentes da velocidade são calculadas primeiramente. Dessa forma, essas equações transformam-se em equações lineares.

Colocando os símbolos de somatória para fora das integrais, temos:

$$\begin{aligned} & \sum_{j=1}^{np} \delta_j \left[\sum_{i=1}^{np} \dot{w}_i \int_{\Omega} N_i N_j d\Omega + \sum_{i=1}^{np} w_i \left[u \int_{\Omega} \frac{\partial N_i}{\partial x} N_j d\Omega + v \int_{\Omega} \frac{\partial N_i}{\partial y} N_j d\Omega \right. \right. \\ & + \frac{1}{Re} \int_{\Omega} \left\{ \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right\} d\Omega + \frac{\Delta t}{2} \int_{\Omega} u \frac{\partial N_j}{\partial x} \left[u \frac{\partial N_i}{\partial x} + v \frac{\partial N_i}{\partial y} \right] d\Omega \\ & \left. \left. + \frac{\Delta t}{2} \int_{\Omega} v \frac{\partial N_j}{\partial y} \left[u \frac{\partial N_i}{\partial x} + v \frac{\partial N_i}{\partial y} \right] d\Omega \right] \right] = 0 \end{aligned} \quad (3.66)$$

$$\sum_{j=1}^{np} \phi_j \left[\sum_{i=1}^{np} \psi_i \left[- \int_{\Omega} \left\{ \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right\} d\Omega + w_i \int_{\Omega} N_i N_j d\Omega \right] \right] = 0 \quad (3.67)$$

$$\sum_{j=1}^{np} \xi_j \left[\sum_{i=1}^{np} u_i \left[\int_{\Omega} N_i N_j d\Omega - \psi_i \int_{\Omega} \frac{\partial N_i}{\partial y} N_j d\Omega \right] \right] = 0 \quad (3.68)$$

$$\sum_{j=1}^{np} \xi_j \left[\sum_{i=1}^{np} v_i \left[\int_{\Omega} N_i N_j d\Omega + \psi_i \int_{\Omega} \frac{\partial N_i}{\partial x} N_j d\Omega \right] \right] = 0 \quad (3.69)$$

$$\begin{aligned} & \sum_{j=1}^{np} \eta_j \left[\sum_{i=1}^{np} \dot{c}_i \int_{\Omega} N_i N_j d\Omega + \sum_{i=1}^{np} c_i \left[u \int_{\Omega} \frac{\partial N_i}{\partial x} N_j d\Omega + v \int_{\Omega} \frac{\partial N_i}{\partial y} N_j d\Omega \right. \right. \\ & + \frac{1}{ReSc} \int_{\Omega} \left\{ \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right\} d\Omega + \frac{\Delta t}{2} \int_{\Omega} u \frac{\partial N_j}{\partial x} \left[u \frac{\partial N_i}{\partial x} + v \frac{\partial N_i}{\partial y} \right] d\Omega \\ & \left. \left. + \frac{\Delta t}{2} \int_{\Omega} v \frac{\partial N_j}{\partial y} \left[u \frac{\partial N_i}{\partial x} + v \frac{\partial N_i}{\partial y} \right] d\Omega \right] \right] = 0 \end{aligned} \quad (3.70)$$

Sabendo que $\sum_{j=1}^{np} \delta_j \neq 0$, $\sum_{j=1}^{np} \phi_j \neq 0$, $\sum_{j=1}^{np} \xi_j \neq 0$ e $\sum_{j=1}^{np} \eta_j \neq 0$ então as equações de governo tornam-se:

$$\begin{aligned} & \sum_{j=1}^{np} \sum_{i=1}^{np} \dot{w}_i \int_{\Omega} N_i N_j d\Omega + \sum_{j=1}^{np} \sum_{i=1}^{np} w_i \left[u \int_{\Omega} \frac{\partial N_i}{\partial x} N_j d\Omega + v \int_{\Omega} \frac{\partial N_i}{\partial y} N_j d\Omega \right. \\ & + \frac{1}{Re} \int_{\Omega} \left\{ \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right\} d\Omega + \frac{\Delta t}{2} \int_{\Omega} u \frac{\partial N_j}{\partial x} \left[u \frac{\partial N_i}{\partial x} + v \frac{\partial N_i}{\partial y} \right] d\Omega \\ & \left. + \frac{\Delta t}{2} \int_{\Omega} v \frac{\partial N_j}{\partial y} \left[u \frac{\partial N_i}{\partial x} + v \frac{\partial N_i}{\partial y} \right] d\Omega \right] = 0 \end{aligned} \quad (3.71)$$

$$\sum_{j=1}^{np} \sum_{i=1}^{np} \psi_i \left[- \int_{\Omega} \left\{ \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right\} d\Omega + w_i \int_{\Omega} N_i N_j d\Omega \right] = 0 \quad (3.72)$$

$$\sum_{j=1}^{np} \sum_{i=1}^{np} u_i \left[\int_{\Omega} N_i N_j d\Omega - \psi_i \int_{\Omega} \frac{\partial N_i}{\partial y} N_j d\Omega \right] = 0 \quad (3.73)$$

$$\sum_{j=1}^{np} \sum_{i=1}^{np} v_i \left[\int_{\Omega} N_i N_j d\Omega + \psi_i \int_{\Omega} \frac{\partial N_i}{\partial x} N_j d\Omega \right] = 0 \quad (3.74)$$

$$\begin{aligned} & \sum_{j=1}^{np} \sum_{i=1}^{np} \dot{c}_i \int_{\Omega} N_i N_j d\Omega + \sum_{j=1}^{np} \sum_{i=1}^{np} c_i \left[u \int_{\Omega} \frac{\partial N_i}{\partial x} N_j d\Omega + v \int_{\Omega} \frac{\partial N_i}{\partial y} N_j d\Omega \right. \\ & + \frac{1}{ReSc} \int_{\Omega} \left\{ \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right\} d\Omega + \frac{\Delta t}{2} \int_{\Omega} u \frac{\partial N_j}{\partial x} \left[u \frac{\partial N_i}{\partial x} + v \frac{\partial N_i}{\partial y} \right] d\Omega \\ & \left. + \frac{\Delta t}{2} \int_{\Omega} v \frac{\partial N_j}{\partial y} \left[u \frac{\partial N_i}{\partial x} + v \frac{\partial N_i}{\partial y} \right] d\Omega \right] = 0 \end{aligned} \quad (3.75)$$

isto é:

$$\begin{aligned} & \sum_{j=1}^{np} \sum_{i=1}^{np} \dot{w}_i \int_{\Omega} N_i N_j d\Omega + \sum_{j=1}^{np} \sum_{i=1}^{np} w_i \left[u \int_{\Omega} \frac{\partial N_i}{\partial x} N_j d\Omega + v \int_{\Omega} \frac{\partial N_i}{\partial y} N_j d\Omega \right. \\ & + \frac{1}{Re} \int_{\Omega} \left\{ \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right\} d\Omega + \frac{\Delta t}{2} \int_{\Omega} u \left[u \frac{\partial N_j}{\partial x} \frac{\partial N_i}{\partial x} + v \frac{\partial N_j}{\partial x} \frac{\partial N_i}{\partial y} \right] d\Omega \\ & \left. + \frac{\Delta t}{2} \int_{\Omega} v \left[u \frac{\partial N_j}{\partial y} \frac{\partial N_i}{\partial x} + v \frac{\partial N_j}{\partial y} \frac{\partial N_i}{\partial y} \right] d\Omega \right] = 0 \end{aligned} \quad (3.76)$$

$$\sum_{j=1}^{np} \sum_{i=1}^{np} \psi_i \left[- \int_{\Omega} \left\{ \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right\} d\Omega + w_i \int_{\Omega} N_i N_j d\Omega \right] = 0 \quad (3.77)$$

$$\sum_{j=1}^{np} \sum_{i=1}^{np} u_i \left[\int_{\Omega} N_i N_j d\Omega - \psi_i \int_{\Omega} \frac{\partial N_i}{\partial y} N_j d\Omega \right] = 0 \quad (3.78)$$

$$\sum_{j=1}^{np} \sum_{i=1}^{np} v_i \left[\int_{\Omega} N_i N_j d\Omega + \psi_i \int_{\Omega} \frac{\partial N_i}{\partial x} N_j d\Omega \right] = 0 \quad (3.79)$$

$$\begin{aligned}
& \sum_{j=1}^{np} \sum_{i=1}^{np} \dot{c}_i \int_{\Omega} N_i N_j d\Omega + \sum_{j=1}^{np} \sum_{i=1}^{np} c_i \left[u \int_{\Omega} \frac{\partial N_i}{\partial x} N_j d\Omega + v \int_{\Omega} \frac{\partial N_i}{\partial y} N_j d\Omega \right. \\
& + \frac{1}{ReSc} \int_{\Omega} \left\{ \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right\} d\Omega + \frac{\Delta t}{2} \int_{\Omega} u \left[u \frac{\partial N_j}{\partial x} \frac{\partial N_i}{\partial x} + v \frac{\partial N_j}{\partial x} \frac{\partial N_i}{\partial y} \right] d\Omega \\
& \left. + \frac{\Delta t}{2} \int_{\Omega} v \left[u \frac{\partial N_j}{\partial y} \frac{\partial N_i}{\partial x} + v \frac{\partial N_j}{\partial y} \frac{\partial N_i}{\partial y} \right] d\Omega \right] = 0
\end{aligned} \quad (3.80)$$

3.5 Semi-Lagrangian Method

Nesta seção discretizaremos as equações de governo no tempo, através da expansão em série de Taylor para a variável em questão a fim de aproximar a derivada temporal. Com o intuito de simplificação, apresentaremos a discretização da equação da vorticidade. Um procedimento semelhante poderá ser feito para a equação de transporte de espécie química (Eq. 2.74). Sendo assim, expandindo os termos da equação da vorticidade (Eq. 2.71), temos:

$$\frac{\partial w}{\partial t} + u \frac{\partial w}{\partial x} + v \frac{\partial w}{\partial y} = \frac{1}{Re} \frac{\partial^2 w}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w}{\partial y^2} \quad (3.81)$$

isto é:

$$\frac{\partial w}{\partial t} = -u \frac{\partial w}{\partial x} - v \frac{\partial w}{\partial y} + \frac{1}{Re} \frac{\partial^2 w}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w}{\partial y^2} \quad (3.82)$$

Multiplicando ambos os lado por $\partial/\partial t$, temos:

$$\frac{\partial}{\partial t} \left[\frac{\partial w}{\partial t} \right] = \frac{\partial}{\partial t} \left[-u \frac{\partial w}{\partial x} - v \frac{\partial w}{\partial y} + \frac{1}{Re} \frac{\partial^2 w}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w}{\partial y^2} \right] \quad (3.83)$$

Desta forma, considerando a expansão de Taylor:

$$w^{n+1} = \sum_{k=0}^{\infty} \frac{\partial^k w^n}{\partial t^k} \frac{\Delta t^k}{k!} \quad (3.84)$$

Desenvolvendo a série, temos:

$$w^{n+1} = w^n + \frac{\partial w^n}{\partial t} \frac{\Delta t}{1!} + \frac{\partial^2 w^n}{\partial t^2} \frac{\Delta t^2}{2!} + \frac{\partial^3 w^n}{\partial t^3} \frac{\Delta t^3}{3!} + \dots \quad (3.85)$$

Caso os termos de ordem superior a dois forem omitidos, a equação fica da forma:

$$w^{n+1} = w^n + \frac{\partial w^n}{\partial t} \Delta t + \frac{\partial^2 w^n}{\partial t^2} \frac{\Delta t^2}{2} + O(\Delta t^3) \quad (3.86)$$

onde $O(\Delta t^3)$ é o erro devido ao truncamento da série. Graficamente, esta aproximação pode ser representada como apresentado na Figure 4, a seguir:

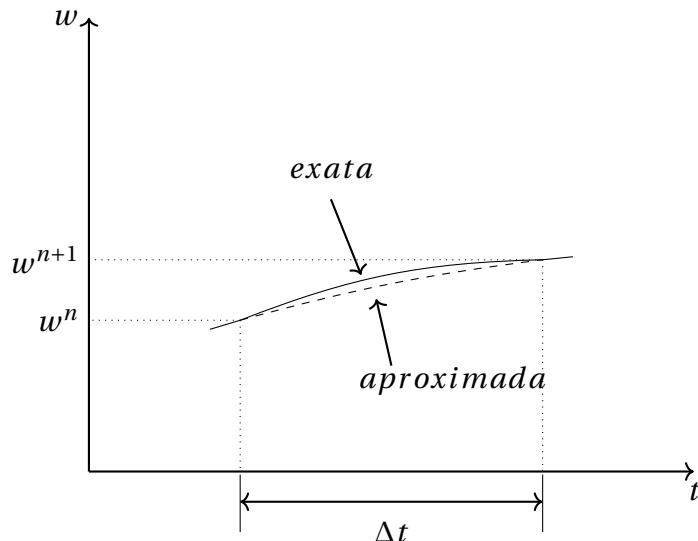


Figure 4: Variação da vorticidade em um passo de tempo

Omitindo o erro do truncamento, a derivada temporal (Eq. 3.86) pode ser aproximada a:

$$w^{n+1} = w^n + \frac{\partial w^n}{\partial t} \Delta t + \frac{\partial^2 w^n}{\partial t^2} \frac{\Delta t^2}{2} \quad (3.87)$$

onde w^{n+1} é a vorticidade que será calculada e w^n é a vorticidade que foi calculada no passo de tempo anterior. Substituindo a equação da vorticidade (Eq. 3.82) e a equação da vorticidade multiplicada pela derivada temporal (Eq. 3.83) na aproximação feita acima,

temos:

$$\begin{aligned} w^{n+1} = w^n + \Delta t & \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial y} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \right] \\ & + \frac{\Delta t^2}{2} \left[\frac{\partial}{\partial t} \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial y} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \right] \right] \end{aligned} \quad (3.88)$$

Assumindo que u e v são constantes, temos:

$$\begin{aligned} w^{n+1} = w^n + \Delta t & \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial y} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \right] \\ & + \frac{\Delta t^2}{2} \left[-u \frac{\partial}{\partial t} \frac{\partial w^n}{\partial x} - v \frac{\partial}{\partial t} \frac{\partial w^n}{\partial y} + \frac{1}{Re} \frac{\partial}{\partial t} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial}{\partial t} \frac{\partial^2 w^n}{\partial y^2} \right] \end{aligned} \quad (3.89)$$

Invertendo as ordens de derivação do último termo, encontramos:

$$\begin{aligned} w^{n+1} = w^n + \Delta t & \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial x} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \right] \\ & + \frac{\Delta t^2}{2} \left[-u \frac{\partial}{\partial x} \frac{\partial w^n}{\partial t} - v \frac{\partial}{\partial y} \frac{\partial w^n}{\partial t} + \frac{1}{Re} \frac{\partial^2}{\partial x^2} \frac{\partial w^n}{\partial t} + \frac{1}{Re} \frac{\partial^2}{\partial y^2} \frac{\partial w^n}{\partial t} \right] \end{aligned} \quad (3.90)$$

Substituindo os termo $\partial w / \partial t$ pela equação de vorticidade (Eq. 3.82), temos:

$$\begin{aligned} w^{n+1} = w^n + \Delta t & \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial x} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \right] \\ & + \frac{\Delta t^2}{2} \left[-u \frac{\partial}{\partial x} \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial y} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \right] \right. \\ & \quad \left. - v \frac{\partial}{\partial y} \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial y} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \right] \right. \\ & \quad \left. + \frac{\partial^2}{\partial x^2} \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial y} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \right] \right. \\ & \quad \left. + \frac{\partial^2}{\partial y^2} \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial y} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \right] \right] \end{aligned} \quad (3.91)$$

Truncando os termos de ordem superior a dois, obtemos:

$$\begin{aligned} w^{n+1} = w^n + \Delta t & \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial x} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \right] \\ & + \frac{\Delta t^2}{2} \left[-u \frac{\partial}{\partial x} \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial y} \right] - v \frac{\partial}{\partial y} \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial y} \right] \right] + O(\Delta t^3) \end{aligned} \quad (3.92)$$

Omitindo novamente o erro de truncamento, possuímos a seguinte equação:

$$\begin{aligned} w^{n+1} = w^n + \Delta t & \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial x} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \right] \\ & + \frac{\Delta t^2}{2} \left[-u \frac{\partial}{\partial x} \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial y} \right] - v \frac{\partial}{\partial y} \left[-u \frac{\partial w^n}{\partial x} - v \frac{\partial w^n}{\partial y} \right] \right] \end{aligned} \quad (3.93)$$

isto é:

$$\begin{aligned} \left[\frac{w^{n+1} - w^n}{\Delta t} \right] + u \frac{\partial w^n}{\partial x} + v \frac{\partial w^n}{\partial y} &= \frac{1}{Re} \frac{\partial^2 w^n}{\partial x^2} + \frac{1}{Re} \frac{\partial^2 w^n}{\partial y^2} \\ & + \frac{\Delta t}{2} u \frac{\partial}{\partial x} \left[u \frac{\partial w^n}{\partial x} + v \frac{\partial w^n}{\partial y} \right] + \frac{\Delta t}{2} v \frac{\partial}{\partial y} \left[u \frac{\partial w^n}{\partial x} + v \frac{\partial w^n}{\partial y} \right] \end{aligned} \quad (3.94)$$

Os dois últimos termos da equação acima são conhecidos como difusão artificial ou difusão numérica e são eles que atuam para a redução das oscilações espúrias que aparecem para Reynolds moderados ou elevados. Outros esquemas são conhecidos na literatura para eliminar essas oscilações espúrias tais como *Petrov-Galerkin* para equações em 1D e *Streamline Upwind Petrov-Galerkin* (SUPG) para equações em 2D ambos em problemas permanentes. Nesses esquemas, as funções bases são modificadas para obter um efeito *upwind*. Para problemas transientes, além do *Taylor-Galerkin* temos: *Semi-Lagrangiano* e *Galerkin Característico*. Os esquemas *Taylor-Galerkin* e *Galerkin Característico* possuem o mesmo resultado quando a variável é escalar como apresentado por Lohner, Morgan e Zienkiewicz (1984) [30].

Na forma vetorial, as equações de governo discretizadas no tempo possuem a forma:

$$\dot{w} + \mathbf{v} \cdot \nabla w = \frac{1}{Re} \nabla^2 w + \frac{\Delta t}{2} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla w] \quad (3.95)$$

$$\nabla^2 \psi = -w \quad (3.96)$$

$$\mathbf{v} = \mathbf{D}\psi \quad (3.97)$$

$$\dot{c} + \mathbf{v} \cdot \nabla c = \frac{1}{ReSc} \nabla^2 c + \frac{\Delta t}{2} \mathbf{v} \cdot \nabla [\mathbf{v} \cdot \nabla c] \quad (3.98)$$

onde \dot{w} e \dot{c} são $[w^{n+1} - w^n]/\Delta t$ e $[c^{n+1} - c^n]/\Delta t$ respectivamente, \mathbf{v} é o vetor velocidade cujas componentes são $\mathbf{v} = [u, v]$ e \mathbf{D} é um operador diferencial com componentes $\mathbf{D} = [\partial/\partial y, -\partial/\partial x]$.

3.6 Mesh Elements

Uma malha computacional pode ser estruturada ou não e a escolha do elemento que constitui esta malha é de vital importância para uma boa precisão da solução. Alguns parâmetros podem influenciar na escolha de um determinado grupo de elementos como por exemplo no caso onde existe uma condição de restrição como é encontrada na equação Navier-Stokes devido o forte acoplamento entre a velocidade e a pressão. Essa restrição é conhecida como *Babuska-Brezzi* [39] [40]. Quando possuímos essa restrição, precisamos ter diferentes números de nós para cada variável no mesmo elemento a fim de possuirmos estabilidade na solução. Sendo assim, precisamos utilizar um *elemento quadrático ou cúbico*. Mas a formulação corrente-voticidade da equação Navier-Stokes não possui a restrição *Babuska-Brezzi* já que não há o acoplamento entre a velocidade e a pressão. Desta forma, o uso de um *elemento linear* não produz instabilidade, podendo ser utilizado sem problemas neste trabalho.

Abaixo apresentaremos a classificação dos elementos quanto à geometria e à ordem do polinômio interpolador conforme apresentado por Anjos (2007) [36]:

- Geometria
 - problemas unidimensionais - Reta
 - problemas bidimensionais - Triangulares e Retangulares
 - problemas tridimensionais - Tetraedrais, hexaedrais e prismáticos
- Ordem do polinômio interpolador
 - grau um - Linear
 - grau dois - Quadrática
 - grau três - Cúbica

Os elementos triangulares são os mais comuns no MEF porque possibilita uma boa discretização de superfícies irregulares devido a sua simplicidade geométrica. Neste trabalho, utilizamos um elemento triangular com o polinômio interpolador de ordem um, isto é, linear.

Abaixo são apresentados alguns elementos triangulares com diferentes ordens do polinômio interpolador:

Elemento triangular linear: Devido sua simplicidade, é o elemento mais utilizado em MEF quando não possuímos restrições. As matrizes elementares analíticas deste elemento são facilmente encontradas na literatura. Como se trata de um elemento linear, a ordem do polinômio interpolador é de grau um. Desta forma, suas funções de interpolação são planas. Este elemento é representado pela Figure 5:

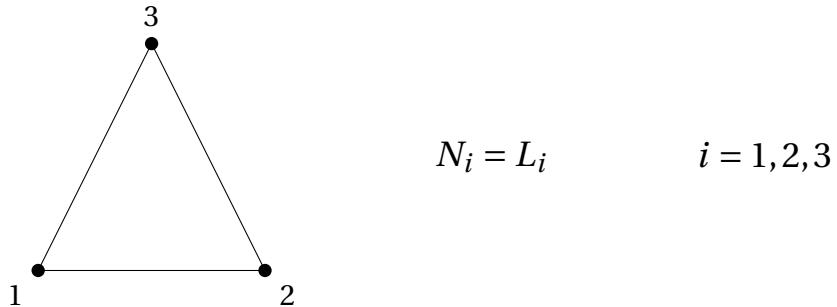


Figure 5: Elemento triangular linear

Elemento triangular quadrático: Geralmente este elemento é usado quando possuímos restrições que impedem o uso do elemento linear ou quando estamos buscando uma melhor aproximação do resultado. As matrizes elementares deste elemento são calculadas pela quadratura gaussiana cujos parâmetros podem ser encontrados na literatura. Como se trata de um elemento quadrático, a ordem do polinômio interpolador é de grau dois. Desta forma, suas funções de interpolação são parabólicas. Este elemento é representado pela Figure 6:

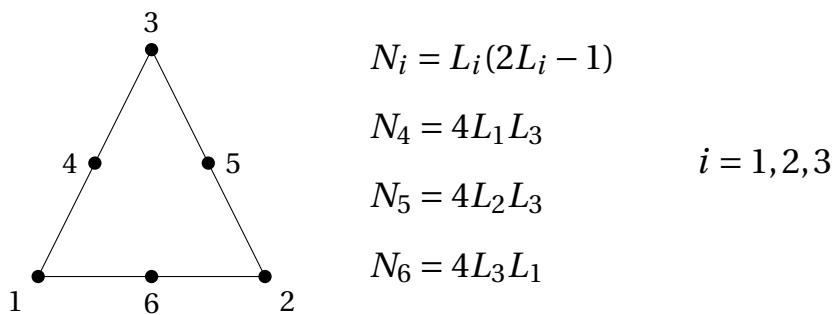


Figure 6: Elemento triangular quadrático

Elemento triangular cúbico: Assim como o elemento quadrático, este elemento é usado quando possuímos restrições que impedem o uso do elemento linear ou quando estamos buscando uma melhor aproximação do resultado. Na literatura, este elemento é conhecido como *elemento MINI*. Suas matrizes elementares também são calculadas pela quadratura

gaussiana. Como se trata de um elemento cúbico, a ordem do polinômio interpolador é de grau três. Desta forma, suas funções de interpolação possuem uma bolha no centro do elemento. Este elemento é representado pela Figure 7:

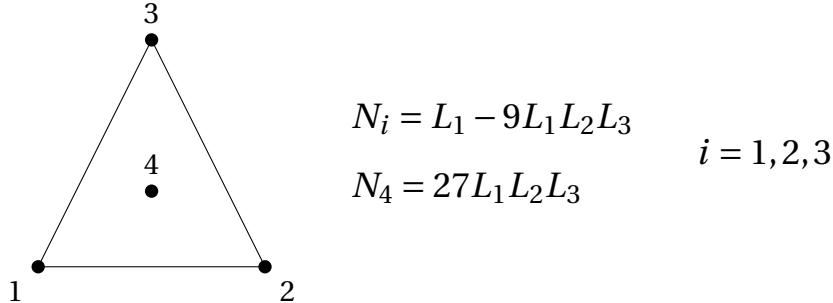


Figure 7: Elemento triangular cúbico

As Eqs (3.76 a 3.80) podem ser representadas matricialmente por:

$$\begin{aligned} M\dot{w} + u \cdot G_x w + v \cdot G_y w + \frac{1}{Re} [K_{xx} + K_{yy}] w \\ + \frac{\Delta t}{2} u [u K_{xx} + v K_{yx}] w + \frac{\Delta t}{2} v [u K_{xy} + v K_{yy}] w = 0 \end{aligned} \quad (3.99)$$

$$- [K_{xx} + K_{yy}] \psi + Mw = 0 \quad (3.100)$$

$$Mu - G_y \psi = 0 \quad (3.101)$$

$$Mv + G_x \psi = 0 \quad (3.102)$$

$$\begin{aligned} M\dot{c} + u \cdot G_x c + v \cdot G_y c + \frac{1}{ReSc} [K_{xx} + K_{yy}] c \\ + \frac{\Delta t}{2} u [u K_{xx} + v K_{xy}] c + \frac{\Delta t}{2} v [u K_{yx} + v K_{yy}] c = 0 \end{aligned} \quad (3.103)$$

onde as matrizes \mathbf{M} , \mathbf{G}_x , \mathbf{G}_y , \mathbf{K}_{xx} , \mathbf{K}_{xy} , \mathbf{K}_{yx} , \mathbf{K}_{yy} , possuem dimensões $\mathbf{np} \times \mathbf{np}$ (isto é, número de nós por número de nós) e são definidas como:

$$\mathbf{M} = \mathbf{A}m^e \quad (3.104)$$

$$\mathbf{G}_x = \mathbf{A}g_x^e \quad (3.105)$$

$$\mathbf{G}_y = \mathbf{A}g_y^e \quad (3.106)$$

$$\mathbf{K}_{xx} = \mathbf{A}k_{xx}^e \quad (3.107)$$

$$\mathbf{K}_{xy} = \mathbf{A}k_{xy}^e \quad (3.108)$$

$$\mathbf{K}_{yx} = \mathbf{A}k_{yx}^e \quad (3.109)$$

$$\mathbf{K}_{yy} = \mathbf{A}k_{yy}^e \quad (3.110)$$

onde \mathbf{A} é um operador de montagem das matrizes elementares nas matrizes globais, respeitando a correspondência entre os índices globais e locais e m^e , g_x^e , g_y^e , k_{xx}^e , k_{xy}^e , k_{yx}^e , k_{yy}^e são as matrizes elementares cuja dimensão para o *elemento triangular linear* é 3x3 e são definidas por:

$$\begin{aligned} m^e &= \int_{\Omega^e} N_i^e N_j^e d\Omega \\ g_x^e &= \int_{\Omega^e} \frac{\partial N_i^e}{\partial x} N_j^e d\Omega \\ g_y^e &= \int_{\Omega^e} \frac{\partial N_i^e}{\partial y} N_j^e d\Omega \\ k_{xx}^e &= \int_{\Omega^e} \frac{\partial N_i^e}{\partial x} \frac{\partial N_j^e}{\partial x} \\ k_{xy}^e &= \int_{\Omega^e} \frac{\partial N_i^e}{\partial x} \frac{\partial N_j^e}{\partial y} \\ k_{yx}^e &= \int_{\Omega^e} \frac{\partial N_i^e}{\partial y} \frac{\partial N_j^e}{\partial x} \\ k_{yy}^e &= \int_{\Omega^e} \frac{\partial N_i^e}{\partial y} \frac{\partial N_j^e}{\partial y} \end{aligned} \quad (3.111)$$

Sendo assim, as equações de governo em sua forma matricial discretizadas segundo o

Método dos Elementos Finitos que usamos neste trabalho foram:

$$\begin{aligned} \frac{M}{\Delta t} w^{n+1} = & \frac{M}{\Delta t} w^n - u \cdot G_x w^n - v \cdot G_y w^n - \frac{1}{Re} [K_{xx} + K_{yy}] w^n \\ & - \frac{\Delta t}{2} u [u K_{xx} + v K_{yx}] w^n - \frac{\Delta t}{2} v [u K_{xy} + v K_{yy}] w^n \end{aligned} \quad (3.112)$$

$$[K_{xx} + K_{yy}] \psi = M w \quad (3.113)$$

$$M u = G_y \psi \quad (3.114)$$

$$M v = -G_x \psi \quad (3.115)$$

$$\begin{aligned} \frac{M}{\Delta t} c^{n+1} = & \frac{M}{\Delta t} c^n - u \cdot G_x c^n - v \cdot G_y c^n - \frac{1}{ReSc} [K_{xx} + K_{yy}] c^n \\ & - \frac{\Delta t}{2} u [u K_{xx} + v K_{yx}] c^n - \frac{\Delta t}{2} v [u K_{xy} + v K_{yy}] c^n \end{aligned} \quad (3.116)$$

4 CÓDIGO NUMÉRICO

4.1 Introdução

Neste capítulo apresentaremos as principais características do código numérico desenvolvido em linguagem Python 2.7 [41] utilizando o paradigma de orientação a objetos com o intuito da reutilização do código em outras simulações no futuro. Todas as classes desenvolvidas são importadas no simulador (*TriSim*) onde é exportado o resultado da simulação numérica conforme apresentado no *Diagrama de Classes* (UML) simplificado da Figure 8. Inicialmente, é apresentado o *script* que realiza a importação da malha computacional para a simulação. Em seguida, a montagem das matrizes globais é feita respeitando a correspondência entre os índices globais e locais. Mais a frente, apresentamos a aplicação das condições de contorno tanto de *Dirichlet* quanto de *Neumann*. E finalmente, é apresentado também, o algoritmo de solução da formulação corrente-vorticidade com a equação de transferência de espécie química.

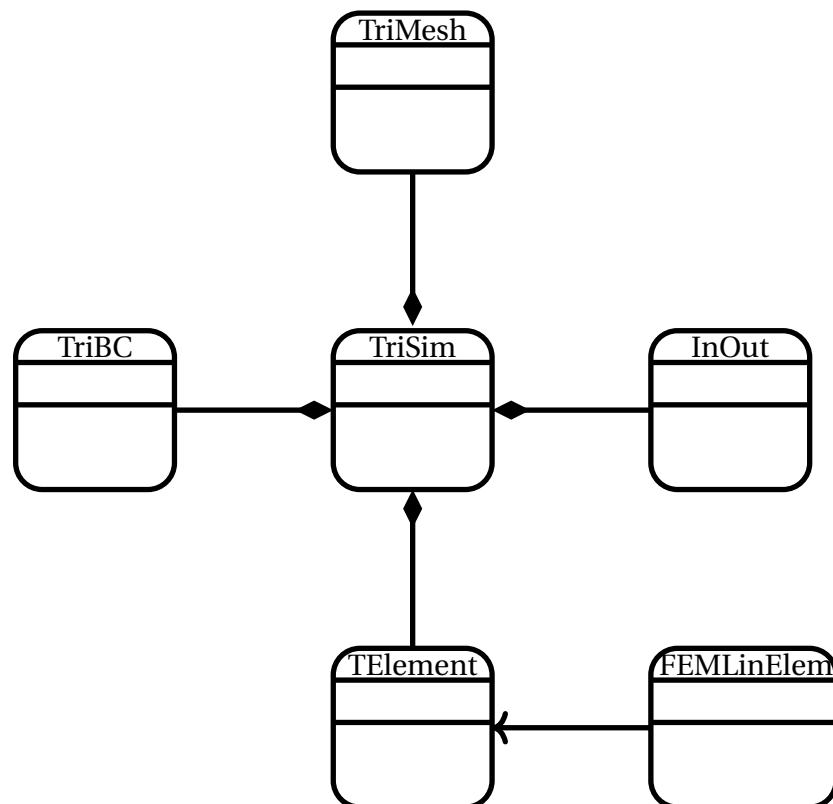


Figure 8: Diagrama de Classes Simplificado

4.2 Importação da Malha

O domínio consiste em uma malha não estruturada gerada pelo software livre *GMSH* proposto por Geuzaine e Remacle (2009) [42] e foi importada à simulação pela classe *TriMesh*. Inicialmente transformamos o arquivo *.msh* em uma lista *Python* pelo script abaixo:

```
malha = []                                | inicialização da lista Python
with open("arquivo.msh") as mesh:
    for line in mesh:                      | loop sobre as linhas do arquivo
        row = line.split()
        malha.append(row[:])                | adicionando a linha
                                                | do arquivo na lista Python
```

Em seguida, esta classe retorna informações importantes para a simulação tais como: *o número de nós do domínio (np)*, *o número de elementos do domínio (ne)*, *os vetores de coordenadas (x e y)*, *a matriz de conectividade (IEN)* e *os nós contidos no contorno do domínio*. A Table 1 apresenta o tempo de processamento para a importação da malha em diversas malhas triangulares lineares não estruturadas.

N. Nós	N. Elementos	Tempo de Processamento (s)
10482	20142	0,6
40819	80005	2,6
249677	495289	16,6
993091	2010501	70,4

Table 1: Tempo de importação para diversas malhas triangulares não estruturadas

4.3 Montagem das Matrizes Globais

Após a importação do arquivo *.msh* foi realizado a montagem das matrizes globais. As mesmas foram inicializadas como matrizes esparsas pela biblioteca *Scipy* [43] e o seguinte *script* foi usado para a montagem:

```

for e in range(0, ne):           | loop sobre os elementos
    linear_element(e)           | montagem das matrizes elementares
                                  | utilizando a quadratura gaussiana

    for i in range(0,3):
        ii = IEN[e][i]

        for j in range(0,3):
            jj = IEN[e][j]

            Kxx[ii,jj] += kxx_element[i][j]      |
            Kxy[ii,jj] += kxy_element[i][j]      |
            Kyx[ii,jj] += kyx_element[i][j]      |
            Kyy[ii,jj] += kyy_element[i][j]      | montagem das matrizes globais
                                              | correspondendo os índices globais
            Gx[ii,jj] += gx_element[i][j]      | e locais
            Gy[ii,jj] += gy_element[i][j]      |
                                              |
            M[ii,jj] += mass_element[i][j]      |

```

A montagem das matrizes elementares é feita pelo módulo *linear_element* cujo parâmetro requerido é o número do elemento. Esse módulo faz parte da classe *TElement* onde utiliza a quadratura gaussiana para o cálculo dos valores das matrizes elementares. Para o elemento triangular linear, é possível a utilização das matrizes elementares analíticas. Para mais detalhe consultar o trabalho de Lewis, Nithiarasu e Seetharamu (2004) [44].

Em seguida, a matriz do lado esquerdo conhecida como *left hand side (LHS)* é criada para as equações da função de corrente, velocidade e concentração respectivamente:

```
LHS_psi = sps.lil_matrix.copy(K)
LHS_vx = sps.lil_matrix.copy(M)
LHS_vy = sps.lil_matrix.copy(M)
LHS_c = sps.lil_matrix.copy(M)/dt
```

A matriz *LHS* para a equação da vorticidade é criada durante o loop do algoritmo de solução a fim de garantir que a mesma será sempre inicializada utilizando as matrizes globais originais. É necessário usarmos a função *copy* porque queremos copiar os valores das matrizes globais e não referencia-los, para mais detalhe consultar o *Scipy Community* [45]. A Table 2 apresenta o tempo de processamento para para a montagem das matrizes globais em diversas malhas triangulares lineares não estruturadas.

N. Nós	N. Elementos	Tempo de Processamento (s)
10482	20142	72,9
40819	80005	254,3
249677	495289	1664,9
993091	2010501	69059,9

Table 2: Tempo de montagem das matrizes globais para diversas malhas triangulares não estruturadas

4.4 Aplicação das Condições de Contorno

Após a montagem das matrizes globais, as condições de contorno são aplicadas. Conforme foi dito na seção 4.2, durante a importação da malha é possível identificarmos os nós que se encontram no contorno do domínio. A condição onde os nós possuem seus valores pré definidos pelo problema em análise é conhecida como *Condição de Dirichlet*. Sendo assim, esses nós não devem ser alterados conforme a simulação acontece. Dessa maneira, o produto entre a coluna da matriz global cujo índice é um nó com condição de contorno

Dirichlet e o seu valor pré definido como condição de contorno é subtraído ao vetor do lado direito da equação de governo. Em seguida, zeramos as linhas e colunas da matriz global que corresponde ao índice de condição de Dirichlet e colocamos o valor de 1 na diagonal principal.

Para exemplificar, consideraremos uma matriz com dimensões ($np \times np$) e o nó 2 como um nó localizado no contorno do domínio onde a condição proposta é de Dirichlet. Desta forma, o seguinte algoritmo é feito conforme apresentado por Anjos (2007) [36]:

1. Localiza-se o nó de condição de contorno na matriz:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1j} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2j} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3j} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nj} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}$$

↑ Identificar a coluna cujo índice é
condição de contorno de Dirichlet

2. Subtrai-se o produto entre a coluna onde está situado o nó da matriz e o seu valor pré definido com o vetor do lado direito da equação:

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1j} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2j} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3j} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nj} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix}$$

↑ Subtrair o produto desta coluna com o
valor de c_2 no lado direito da equação

isto é,

$$\begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1j} & \cdots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2j} & \cdots & a_{2n} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3j} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ a_{n1} & a_{n2} & a_{n3} & \cdots & a_{nj} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix} - \underbrace{\begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \\ \vdots \\ a_{n2} \end{bmatrix}}_{bc_dirichlet} * c_2$$

- 3. Preenche-se com zeros a coluna e a linha da matriz correspondente ao nó de condição de contorno:**

$$\begin{bmatrix} a_{11} & 0 & a_{13} & \cdots & a_{1j} & \cdots & a_{1n} \\ 0 & 0 & 0 & \cdots & 0 & \cdots & 0 \\ a_{31} & 0 & a_{33} & \cdots & a_{3j} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ a_{n1} & 0 & a_{n3} & \cdots & a_{nj} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix} - \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \\ \vdots \\ a_{n2} \end{bmatrix} * c_2$$

- 4. Coloca-se 1 na diagonal principal da matriz cujo índice é o nó de condição de contorno:**

$$\begin{bmatrix} a_{11} & 0 & a_{13} & \cdots & a_{1j} & \cdots & a_{1n} \\ 0 & 1 & 0 & \cdots & 0 & \cdots & 0 \\ a_{31} & 0 & a_{33} & \cdots & a_{3j} & \cdots & a_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ a_{n1} & 0 & a_{n3} & \cdots & a_{nj} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{bmatrix} - \begin{bmatrix} a_{12} \\ a_{22} \\ a_{32} \\ \vdots \\ a_{n2} \end{bmatrix} * c_2$$

- 5. Localiza-se o próximo nó e executa-se o passo novamente.**

A implementação deste algoritmo foi realizado pelo seguinte *script*:

```

for mm in ibc:                                | loop sobre os nós do contorno
    bc_dirichlet -= LHS[:,mm]*bc_1[mm]        | passo 2
    LHS[:,mm] = 0.0                            | passo 3 - zerar colunas
    LHS[mm,:] = 0.0                            | passo 3 - zerar linhas
    LHS[mm,mm] = 1.0                          | passo 4 - 1 na diagonal principal
    bc_dirichlet[mm] = bc_1[mm]                | imputando o valor da condição
                                                | de Dirichlet no índice
                                                | correspondente

```

onde *ibc* é uma lista que contém todos os nós do contorno cuja condição é de Dirichlet e *bc_1* é um vetor auxiliar com dimensão *np* onde o valor da condição de Dirichlet é imputada em cada índice correspondente. O símbolo `-=` garante que a contribuição de cada nó cuja condição seja de Dirichlet seja computada. Este procedimento deverá ser realizado para cada um das *LHS*. A Table 3 apresenta o tempo de processamento para a aplicação das condições de contorno de *Dirichlet* em diversas malhas triangulares lineares não estruturadas.

N. Nós	N. Elementos	Tempo de Processamento (s)
10482	20142	6,8
40819	80005	37,5
249677	495289	467,7
993091	2010501	3720,6

Table 3: Tempo processamento para as condições de contorno para diversas malhas triangulares não estruturadas

Outro tipo de condição de contorno muito comum é aquela onde existe um fluxo nos contornos do domínio. Essa condição de contorno é conhecida como *Condição de Neumann* e na formulação variacional é chamada de *Condição Natural*. Diferente da condição de Dirichlet, esse tipo de condição de contorno não afeta a matriz global do lado esquerdo quando o fluxo é constante. Devemos apenas somar a sua contribuição no vetor do lado direito da equação, isto é:

$$\begin{bmatrix}
 a_{11} & 0 & a_{13} & \cdots & a_{1j} & \cdots & a_{1n} \\
 0 & 1 & 0 & \cdots & 0 & \cdots & 0 \\
 a_{31} & 0 & a_{33} & \cdots & a_{3j} & \cdots & a_{3n} \\
 \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
 a_{n1} & 0 & a_{n3} & \cdots & a_{nj} & \cdots & a_{nn}
 \end{bmatrix}
 \begin{bmatrix}
 c_1 \\
 c_2 \\
 c_3 \\
 \vdots \\
 c_n
 \end{bmatrix}
 =
 \begin{bmatrix}
 b_1 \\
 b_2 \\
 b_3 \\
 \vdots \\
 b_n
 \end{bmatrix}
 -
 \begin{bmatrix}
 a_{12} \\
 a_{22} \\
 a_{32} \\
 \vdots \\
 a_{n2}
 \end{bmatrix}
 * c_2
 +
 \begin{bmatrix}
 ne_1 \\
 ne_2 \\
 ne_3 \\
 \vdots \\
 ne_n
 \end{bmatrix}$$

bc_dirichlet
 bc_neumann

Como foi mencionado no capítulo 3, possuímos apenas condição de Dirichlet neste trabalho. A seguir, porém, apresentaremos a implementação desse tipo de condição. A fim de exemplificar, consideraremos o termo de contorno da equação 3.24, isto é:

$$\frac{1}{ReSc} \int_{\Gamma} \eta \nabla c \cdot \mathbf{n} d\Gamma \quad (4.1)$$

onde ∇c é o fluxo que será considerado constante. Após a discretização pela formulação de Galerkin, possuímos a seguinte expressão:

$$\frac{1}{ReSc} \int_{\Gamma} N_j \nabla c \cdot \mathbf{n} d\Gamma \quad (4.2)$$

isto é:

$$\frac{1}{ReSc} \left[\frac{\text{length} \nabla c}{2} \right] \quad (4.3)$$

onde a variável *length* é o comprimento da aresta do elemento. Considerando um domínio bidimensional onde i é um nó no contorno deste domínio e $i - 1$ e $i + 1$ são seus vizinhos neste contorno, as arestas do nó i podem ser representadas por:

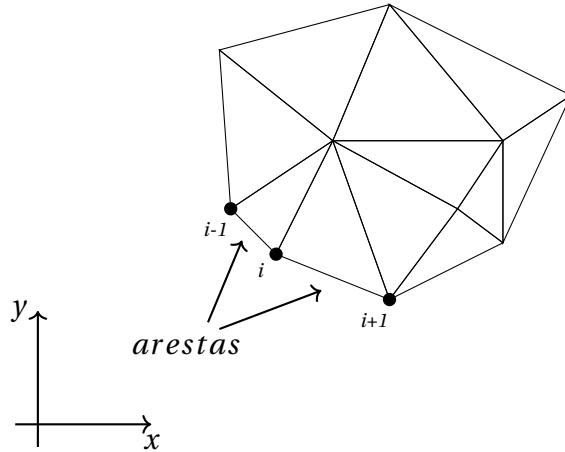


Figure 9: Arestas vizinhas de um nó

onde a aresta à esquerda do nó i é constituída pelos nós $i - 1$ e i , enquanto a aresta à direita é constituída pelos nós i e $i + 1$. Desta maneira podemos observar que o nó i recebe contribuição das aresta a sua esquerda e a sua direita. O script a seguir é usado para a implementação da condição de contorno de Neumann quando requerida:

```

for i in range(0, len(neumann_edges)):      | loop sobre as arestas neumann

    p1 = neumann_edges[i][1]                  | os nós que constituem
    p2 = neumann_edges[i][2]                  | uma aresta

    x = x[p1] - x[p2]                      | calculo do comprimento
    y = y[p1] - y[p2]                      | de uma aresta
    length = numpy.sqrt(x**2 + y**2)        | 

    bc_neumann[p1] += (length*nabla_c) / 2. | imputando o valor da condição
    bc_neumann[p2] += (length*nabla_c) / 2. | de Neumann no índice
                                              | correspondente.

```

onde $neumann_edges$ é uma lista que contém os nós presentes em uma aresta cuja condição é de Neumann, $p1$ e $p2$ são os nós presentes na aresta, x e y são as coordenadas de cada nó,

length é o comprimento da aresta, *nabla_c* é o fluxo adimensional modelado no problema físico e *numpy* é uma biblioteca numérica do *Python* no qual estamos usando a função da raiz quadrada (*numpy.sqrt*). O símbolo $+=$ garante que a contribuição das aresta à esquerda e à direita seja computada.

4.5 Algoritmo de Solução

Uma das grandes dificuldades da implementação da formulação corrente-vorticidade se encontra no algoritmo de solução e a implementação das condições de contorno da vorticidade. Resumidamente, o algoritmo de solução é:

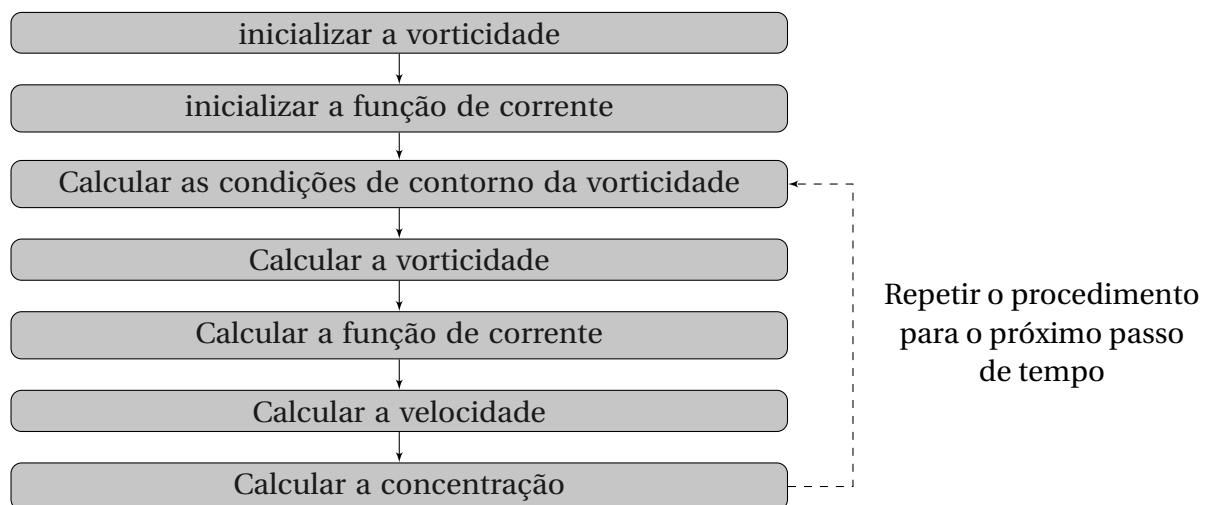


Figure 10: Algoritmo de solução da formulação corrente-vorticidade com transporte de espécie química

Com o intuito de facilitar a implementação do mesmo em outra pesquisa, descreveremos cada passo do algoritmo detalhadamente. As equações estão em sua forma matricial:

1. Inicializar a vorticidade com a equação:

$$Mw = G_x v - G_y u$$

2. Inicializar a função de corrente com a equação:

$$[K_{xx} + K_{yy}] \psi = Mw$$

É necessário aplicar as condições de contorno de ψ na matriz a esquerda da equação zerando suas linhas e colunas e a contribuição das colunas dos índices de contorno no vetor a direita da equação, conforme explicado na seção 4.4.

3. Calcular as condições de contorno da vorticidade utilizando a equação:

$$Mw = G_xv - G_yu$$

Após resolvemos esta equação, possuímos os valores de w para todos os nós do domínio, mas usaremos apenas os nós do contorno para zerar as linhas e as colunas da matriz da equação da vorticidade e sua contribuição no lado direito. Deve-se garantir que a matriz LHS seja inicializada em sua forma original em cada passo de tempo. Para isso, é feito a cada passo de tempo:

```
LHS_w = sps.lil_matrix.copy(M)/dt
```

O script para zerar as linhas e as colunas é semelhante à aplicação da condição de Dirichlet que foi explicado na seção 4.4, exceto à utilização do vetor auxiliar bc_1 que foi substituído pelo w calculado na equação $Mw = G_xv - G_yu$

```
for mm in ibc:                      | loop sobre os nós do contorno de w
    bc_dirichlet = LHS[:,mm]*w[mm]   | o vetor bc_1 é substituído por w
    LHS[:,mm] = 0.0
    LHS[mm,:] = 0.0
    LHS[mm,mm] = 1.0
    bc_dirichlet[mm] = w[mm]         | o vetor bc_1 é substituído por w
```

4. Calcular a vorticidade pela equação:

$$\begin{aligned} \frac{M}{\Delta t}w^{n+1} &= \frac{M}{\Delta t}w^n - u \cdot G_x w^n - v \cdot G_y w^n - \frac{1}{Re} [K_{xx} + K_{yy}] w^n \\ &\quad - u \frac{\Delta t}{2} [u K_{xx} + v K_{yx}] w^n - v \frac{\Delta t}{2} [u K_{xy} + v K_{yy}] w^n \end{aligned}$$

onde w^n é a vorticidade calculada no passo de tempo anterior e w^{n+1} é a vorticidade que será calculada no passo de tempo em análise. É necessário aplicar as condições de contorno de w na matriz a esquerda da equação zerando suas linhas e colunas e a contribuição das colunas dos índices de contorno no vetor a direita da equação, como foi explicado no passo 3.

5. Calcular a função de corrente pela equação:

$$\left[K_{xx} + K_{yy} \right] \psi = Mw$$

É necessário aplicar as condições de contorno de ψ na matriz a esquerda da equação zerando suas linhas e colunas e a contribuição das colunas dos índices de contorno no vetor a direita da equação, conforme explicado na seção 4.4.

6. Calcular a velocidade pela equação:

$$Mu = G_y \psi$$

$$Mv = -G_x \psi$$

É necessário aplicar as condições de contorno de u e v em suas respectivas matrizes a esquerda de cada equação zerando suas linhas e colunas e a contribuição das colunas dos índices de contorno no vetor a direita de cada equação, conforme explicado na seção anterior.

7. Calcular a concentração pela equação:

$$\begin{aligned} \frac{M}{\Delta t} c^{n+1} &= \frac{M}{\Delta t} c^n - u \cdot G_x c^n - v \cdot G_y c^n - \frac{1}{ReSc} \left[K_{xx} + K_{yy} \right] c^n \\ &\quad - u \frac{\Delta t}{2} [u K_{xx} + v K_{yx}] c^n - v \frac{\Delta t}{2} [u K_{xy} + v K_{yy}] c^n \end{aligned}$$

Onde c^n é a concentração calculada no passo de tempo anterior e c^{n+1} é a concentração que será calculada no passo de tempo em análise. É necessário aplicar as condições de contorno de c na matriz a esquerda da equação zerando suas linhas e colunas e a contribuição das colunas dos índices de contorno no vetor a direita da equação, conforme explicado na seção anterior.

8. Retornar ao passo 3 e repetir o procedimento para outro passo de tempo.

Os passos 1 e 2 ficam fora do *loop* do tempo, enquanto os passos de 3 a 7 encontram-se dentro do *loop*. O procedimento para zerar as linhas e as colunas das matrizes globais pode ser feito antes do *loop*, exceto para o caso da vorticidade em que a cada passo de tempo devemos zerar as linhas e as colunas das matrizes globais e atribuir a contribuição dessas colunas no vetor a direita da equação.

A seguir será apresentado o *script* usado na solução da equação da vorticidade. A mesma ideia foi realizada para cada equação de governo, alterando apenas o vetor do lado direito e as contribuições das condições de contorno. Foi utilizado um método iterativo de solução para sistemas lineares conhecido como *Gradientes Conjugados*.

```
RHS = sps.lil_matrix.dot(np.copy(M)/dt,w) \
    - np.multiply(vx,sps.lil_matrix.dot(Gx,w)) \
    - np.multiply(vy,sps.lil_matrix.dot(Gy,w)) \
    - (1.0/Re)*sps.lil_matrix((Kxx+Kyy),w) \
    - (dt/2.0)*np.multiply(u,(np.multiply(u,sps.lil_matrix.dot(Kxx,w)) \
        + np.multiply(v,sps.lil_matrix.dot(Kyx,w)))) \
    - (dt/2.0)*np.multiply(v,(np.multiply(u,sps.lil_matrix.dot(Kxy,w)) \
        + np.multiply(v,sps.lil_matrix.dot(Kyy,w)))) \
RHS = RHS + (1/Re)*bc_neumann
RHS = np.multiply(RHS,bc_2)
RHS = RHS + bc_dirichlet

w = scipy.sparse.linalg.cg(LHS,RHS,w, maxiter=1.0e+05, tol=1.0e-05)
w = w[0].reshape((len(w[0]),1))
```

Onde *RHS* é o vetor do lado direito da equação e significa *right hand side* e *bc_2* é um vetor auxiliar no qual garante que somente os nós sem condição de Dirichlet sejam resolvidos. Ele consiste em um vetor com dimensões *np* onde possui o valor de 1 nos índices cujos nós não possuem condição de Dirichlet e o valor 0 nos índices restantes, isto é, os nós que possuem condição de Dirichlet. Vale ressaltar que o vetor *bc_2* é diferente para cada equação já que os

contornos cuja condição é de Dirichlet variam de equação para equação, ou seja, o vetor bc_2 da equação da vorticidade é diferente da equação de concentração. O primeiro bloco do *script* acima consiste no lado direito da equação (3.112). O segundo bloco refere-se a contribuição das condições de Neumann (para esta simulação é nula) e de Dirichlet, além da aplicação do vetor auxiliar bc_2 . O terceiro bloco consiste na solução da equação pelo método iterativo dos *Gradientes Conjugados*.

5 VALIDAÇÃO DO CÓDIGO NUMÉRICO

5.1 Introdução

Apresentaremos neste capítulo os resultados obtidos de quatro casos com a simulação numérica da equação de Navier-Stokes utilizando a formulação corrente-vorticidade com a equação de transporte de espécie química onde possuímos escoamentos bidimensionais incompressíveis e monofásicos para todos os casos. A primeira seção trata-se do *Escoamento de Couette* e a solução numérica é comparada com a solução analítica. Já a segunda a seção trata-se do *Escoamento de Poiseuille* e a solução numérica também é comparada com a solução analítica. A terceira seção refere-se ao escoamento de *Poiseuille* em meio domínio, onde a condição de livre escorregamento é aplicada sobre o eixo de simetria. A quarta seção refere-se ao escoamento em uma cavidade com tampa deslizante (*lid-driven cavity flow*) e a solução é comparada com os resultados apresentados por Ghia et al. (1982) [7] e Marchi et al. (2009) [8]. Já na quinta seção é apresentado a comparação dos esquemas Galerkin e Taylor-Galerkin do transporte de um escalar submetido a um escoamento puramente convectivo.

Todas as simulações numéricas foram realizadas nos computadores do *Laboratório de Ensaios Numéricos (LEN)* do *Grupo de Estudos e Simulações Ambientais em Reservatórios (GESAR)* com a seguinte configuração:

- AMD FX-8350 4GHz com 8 núcleos, 32Gb de Memória RAM, 1000Gb de HD. Sistema operacional LINUX Ubuntu 16.04 LTS, utilizando a linguagem Python 2.7

5.2 Escoamento de Couette

Um escoamento monofásico, permanente e plenamente desenvolvido de um fluido newtoniano e incompressível entre placas horizontais paralelas onde a placa inferior se desloca com velocidade U_{bottom} enquanto a placa superior se desloca com velocidade U_{top} é conhecido como *Escoamento de Couette*. A Figure 11 apresenta esquematicamente este escoamento e o perfil do campo de velocidade esperado.

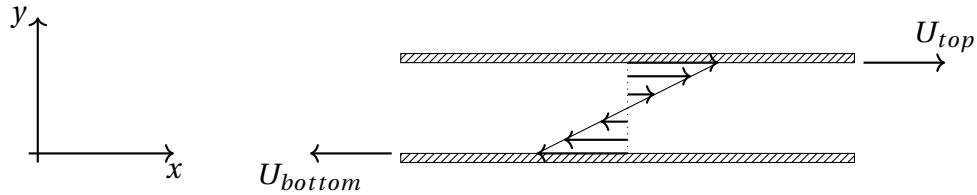


Figure 11: Escoamento de Couette

O perfil de velocidade que este escoamento adquire é dado pela equação abaixo:

$$u = [U_{top} - U_{bottom}] \frac{y}{L} + U_{bottom} \quad (5.1)$$

onde U_{top} é a velocidade que a placa superior se desloca e seu valor é $U_{top} = 1$, U_{bottom} é a velocidade que a placa inferior se desloca e seu valor é $U_{bottom} = -1$, L é a largura não dimensional entre as placas e seu valor é $L = 1$ e y é a distância entre as placas e varia entre $y = [0, 1]$. O domínio foi discretizado utilizando uma malha triangular linear com 3835 nós e 7299 elementos.

As condições de contorno utilizadas foram:

- *condição de entrada:* nenhum valor é especificado. As derivadas das componentes tangencial e normal da velocidade e da função de corrente possuem o valor nulo, isto é, $\partial u / \partial n = 0$, $\partial v / \partial n = 0$ e $\partial \psi / \partial n = 0$ respectivamente.
- *condição de movimentação da parede:* esta condição é utilizada na placa superior e inferior, onde todas as componentes da velocidade e da função de corrente são especificadas. Para a parede superior, $u = U_{top}$, $v = 0$ e $\psi = 0$, onde $U_{top} = 1$. Para a parede inferior, $u = U_{bottom}$, $v = 0$ e $\psi = 0$, onde $U_{bottom} = -1$.
- *condição de saída:* assim como na entrada, nenhum valor é especificado. As derivadas das componentes tangencial e normal da velocidade e da função de corrente possuem o valor nulo, isto é, $\partial u / \partial n = 0$, $\partial v / \partial n = 0$ e $\partial \psi / \partial n = 0$ respectivamente.

A Figure 12 apresenta a evolução do perfil de velocidade no tempo quando o $Re = 100$, além do comparativo entre a solução numérica e a solução analítica no estado permanente do problema proposto. É possível observar que a solução numérica converge para a solução analítica quando o escoamento torna-se permanente.

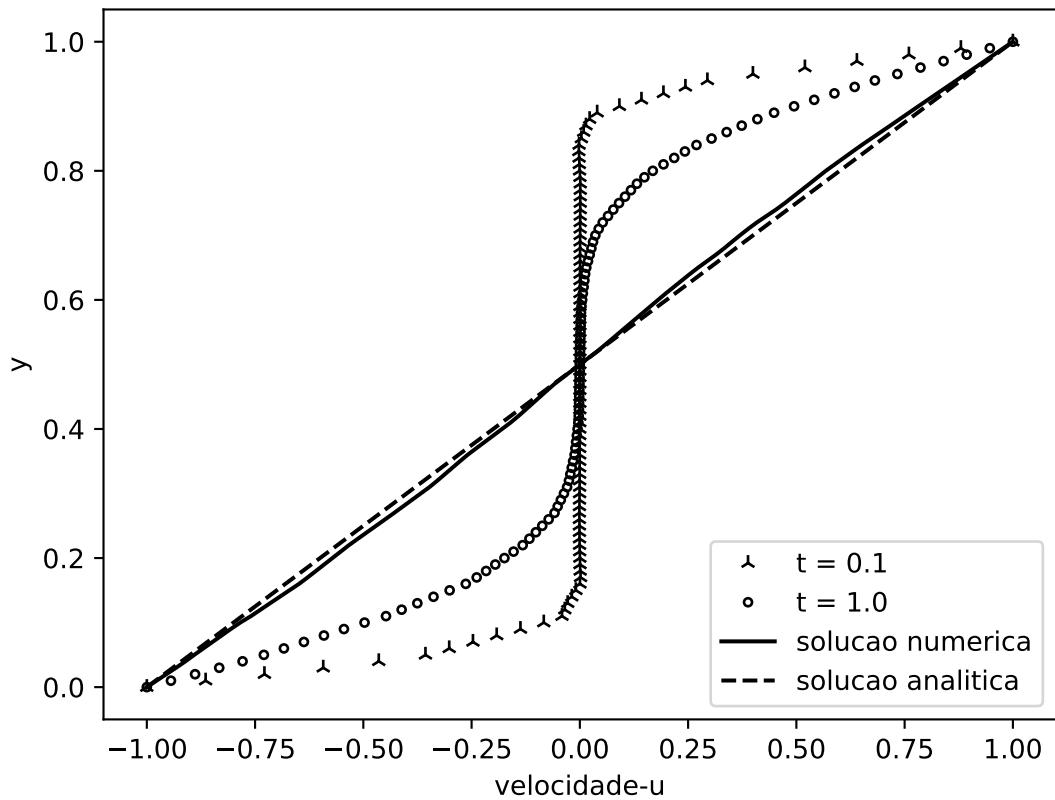


Figure 12: Evolução do perfil de velocidade no tempo para $Re = 100$ e a comparação da solução numérica com a solução analítica para o Escoamento de Couette.

5.3 Escoamento de Poiseuille

Um escoamento monofásico, permanente e plenamente desenvolvido de um fluido newtoniano e incompressível entre placas horizontais paralelas e imóveis é mantido em virtude de um gradiente de pressão $\partial p / \partial x$ imposto conforme mencionado por Pontes e Mangiavacchi (2016) [32]. Este escoamento é conhecido como *Escoamento de Poiseuille*. A Figure 13 apresenta esquematicamente este escoamento e o perfil do campo de velocidade esperado.

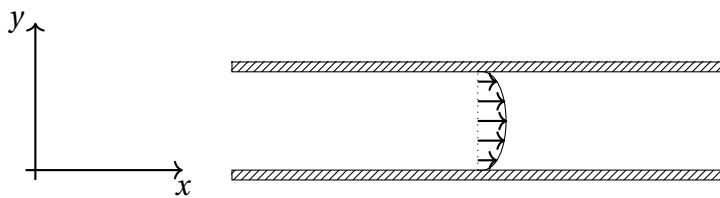


Figure 13: Escoamento de Poiseuille

O perfil de velocidade que este escoamento adquire é dado pela equação abaixo:

$$u = \frac{4u_{max}}{L^2} y[L - y] \quad (5.2)$$

Onde u_{max} é a velocidade máxima e seu valor é $u_{max} = 1.5$, L é a largura não dimensional entre as placas e seu valor é $L = 1$ e y é a distância entre as placas e varia entre $y = [0, 1]$. O domínio foi discretizado utilizando uma malha triangular linear com 3835 nós e 7299 elementos.

As condições de contorno utilizadas foram:

- *condição de entrada*: a componente normal da velocidade $v = 0$ enquanto a componente tangencial da velocidade é $u = 1$. A função de corrente também é especificada e seu valor é definido segundo a equação da continuidade para um fluido incompressível. Dessa forma, seu valor será $\psi = y$.
- *condição de não escorregamento*: esta condição é utilizada nas placas, onde todas as componentes da velocidade são especificadas com os valores $u = 0$ and $v = 0$. A função de corrente também é especificado com os valores $\psi = 1$ na parede superior e $\psi = 0$ na parede inferior.

- *condição de saída:* O valor da função de corrente é especificado $\psi = y$. As derivadas das componentes tangencial e normal da velocidade possuem o valor nulo, isto é, $\partial u / \partial n = 0$ e $\partial v / \partial n = 0$ respectivamente.

A Figure 14 apresenta a evolução do perfil de velocidade no tempo quando o $Re = 100$, além do comparativo entre a solução numérica e a solução analítica no estado permanente do problema proposto.

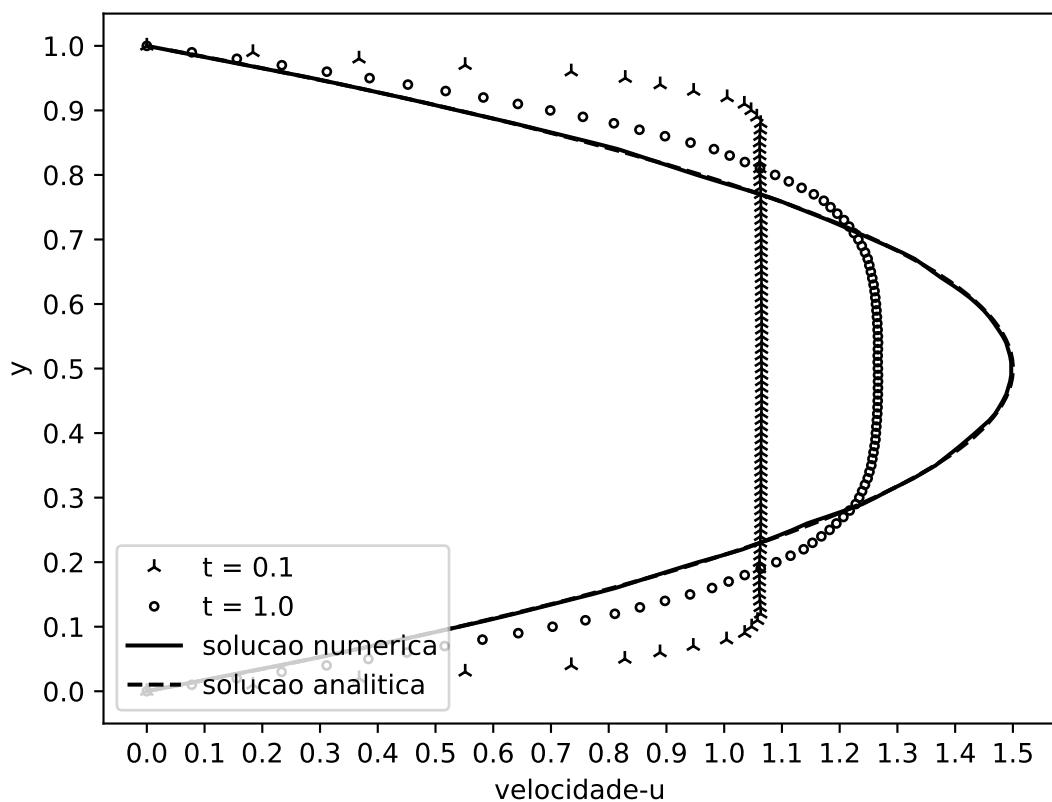


Figure 14: Evolução do perfil de velocidade no tempo e a comparação da solução numérica no estado permanente com a solução analítica para o Escoamento de Poiseuille.

A Table 4 apresenta o erro relativo entre a solução numérica e a solução analítica para diversas malhas não estruturadas, variando entre 100 a 25600 elementos triangulares lineares. Para a malha com 7299 elementos como no caso deste teste, o erro relativo estimado para o campo de velocidade está entre as faixas 0,49% e 0,13%.

N. Elementos	Erro (%)
100	25,00
400	7,27
1600	1,94
6400	0,49
25600	0,13

Table 4: Erro relativo da solução numérica para diferentes malhas não estruturadas

O erro relativo foi estimado como:

$$Error = \sqrt{\frac{\sum (v_n - v_a)^2}{\sum |v_a|^2}} \quad (5.3)$$

onde v_n é o campo da velocidade numérica e v_a é o campo da velocidade analítica.

A Figure 15 apresenta o erro relativo da solução numérica com as curvas de convergência de primeira e segunda ordem em uma escala logarítmica. Como pode ser observado, o erro da solução numérica para diferentes números de elementos triangulares lineares possui a forma de convergência de primeira ordem. Dessa forma, ao aumentar o número de elementos, o erro relativo da solução numérica regredie linearmente.

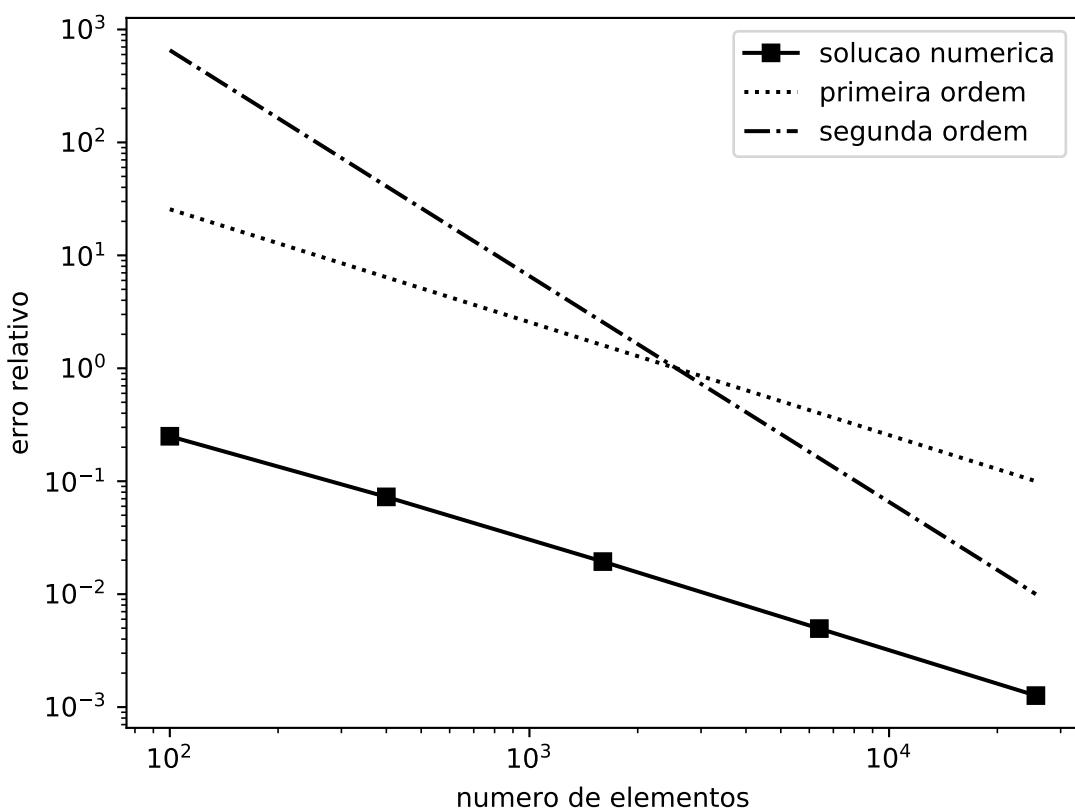


Figure 15: Ordem de convergência em escala logarítmica. É estimado que o erro relativo da solução numérica possui convergência de primeira ordem.

5.4 Escoamento de Poiseuille em Meio Domínio

Nesta seção é apresentado a simulação do escoamento de *Poiseuille* na metade do domínio. Dessa forma, a condição de contorno de superfície livre de escorregamento é necessária no eixo de simetria. A Figure 16 apresenta esquematicamente este escoamento com o eixo de simetria especificado e o perfil do campo de velocidade esperado.

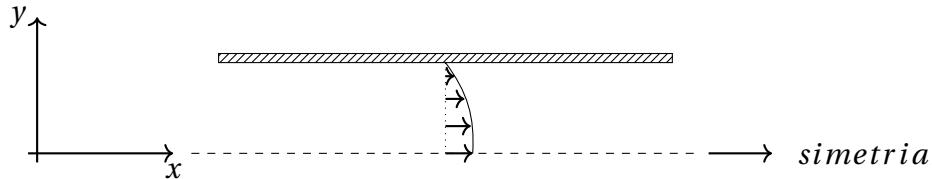


Figure 16: Escoamento de Poiseuille em Meio Domínio

O perfil de velocidade que este escoamento adquire é dado pela equação abaixo:

$$u = u_{max} \left[1 - \frac{y^2}{L^2} \right] \quad (5.4)$$

onde u_{max} é a velocidade máxima e seu valor é $u_{max} = 1.5$, L é a largura não dimensional entre a placa e o eixo de simetria, seu valor é $L = 1$ e y é a distância entre a placas e o eixo de simetria, a mesma varia entre $y = [0, 1]$. O domínio foi discretizado utilizando uma malha triangular linear com 3835 nós e 7299 elementos.

As condições de contorno utilizadas foram:

- *condição de entrada:* a componente normal da velocidade $v = 0$ enquanto a componente tangencial da velocidade é $u = 1$. A função de corrente também é especificada e seu valor é definido segundo a equação da continuidade para um fluido incompressível. Dessa forma, seu valor será $\psi = y$.
- *condição de não escorregamento:* esta condição é utilizada na placa superior, onde todas as componentes da velocidade são especificadas com os valores $u = 0$ e $v = 0$. A função de corrente também é especificado com o valor $\psi = 1$.
- *condição de saída:* O valor da função de corrente é especificado $\psi = y$. As derivadas das componentes tangencial e normal da velocidade possuem o valor nulo, isto é, $\partial u / \partial n = 0$ e $\partial v / \partial n = 0$ respectivamente.

- *condição de livre escorregamento:* esta condição é utilizada no eixo de simetria. A componente normal da velocidade e a função de corrente possuem seus valores especificados, tais como $v = 0$ e $\psi = 0$ respectivamente. A derivada da componente tangencial da velocidade possui o valor nulo $\partial u / \partial n = 0$.

A Figure 17 apresenta a evolução do perfil de velocidade no tempo quando o $Re = 100$, além do comparativo entre a solução numérica e a solução analítica no estado permanente do problema proposto. É possível observar um pequeno desvio entre a solução numérica e a solução analítica próximo ao eixo de simetria.

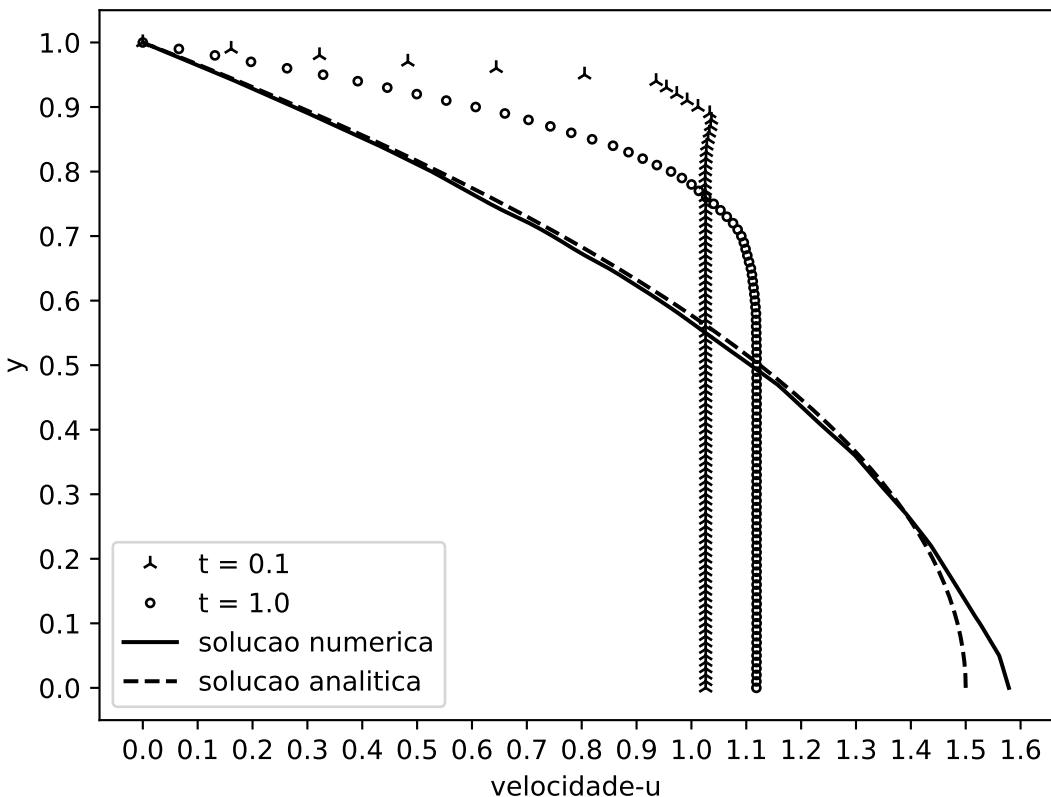


Figure 17: Evolução do perfil de velocidade no tempo para $Re = 100$ e a comparação da solução numérica com a solução analítica para o Escoamento de Poiseuille em Meio Domínio.

5.5 Escoamento em uma Cavidade com Tampa Móvel

Um escoamento em uma cavidade onde as paredes laterais e inferior permanecem imóveis e a tampa se desloca com velocidade constante tal como $U_{top} = 1$ é conhecido como *Escoamento em uma Cavidade de Tampa Móvel* (*lid-driven cavity flow*). A Figure 18 apresenta esquematicamente este escoamento e o perfil do campo de velocidade esperado.

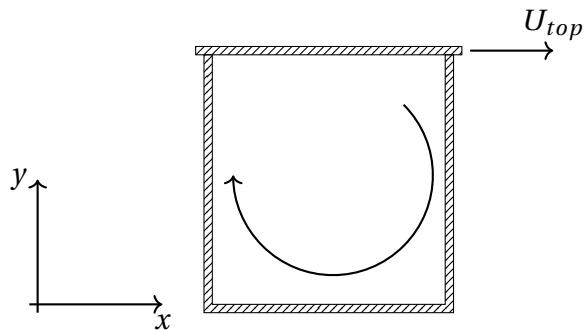


Figure 18: Escoamento em uma Cavidade com tampa móvel

Foram simulados os escoamentos com os seguintes número de Reynolds (Re): 10, 100, 400 e 1000. Os resultados obtidos foram comparados com Ghia et al. (1982) [7] e Marchi et al. (2009) [8]. O domínio foi discretizado utilizando uma malha triangular linear com 1563 nós e 2988 elementos.

As condições de contorno utilizadas foram:

- *condição de não escorregamento*: esta condição é utilizada nas placas laterais e inferior, onde todas as componentes da velocidade são especificadas com os valores $u = 0$ e $v = 0$. A função de corrente também é especificado com o valor de $\psi = 0$.
- *condição de movimentação da parede*: esta condição é utilizada na placa superior, onde todas as componentes da velocidade são especificadas com os valores $u = 1$ e $v = 0$. A função de corrente também é especificado com o valor de $\psi = 0$.

As Figure 19 e Figure 20 apresentam o perfil de u e de v , respectivamente, em regime permanente para vários números de Reynolds. Os resultados obtidos são comparados com os resultados de Ghia et al. (1982) [7] e Marchi et al. (2009) [8]. Na Figure 21, é apresentado os contornos da função de corrente para os Reynolds analisados.

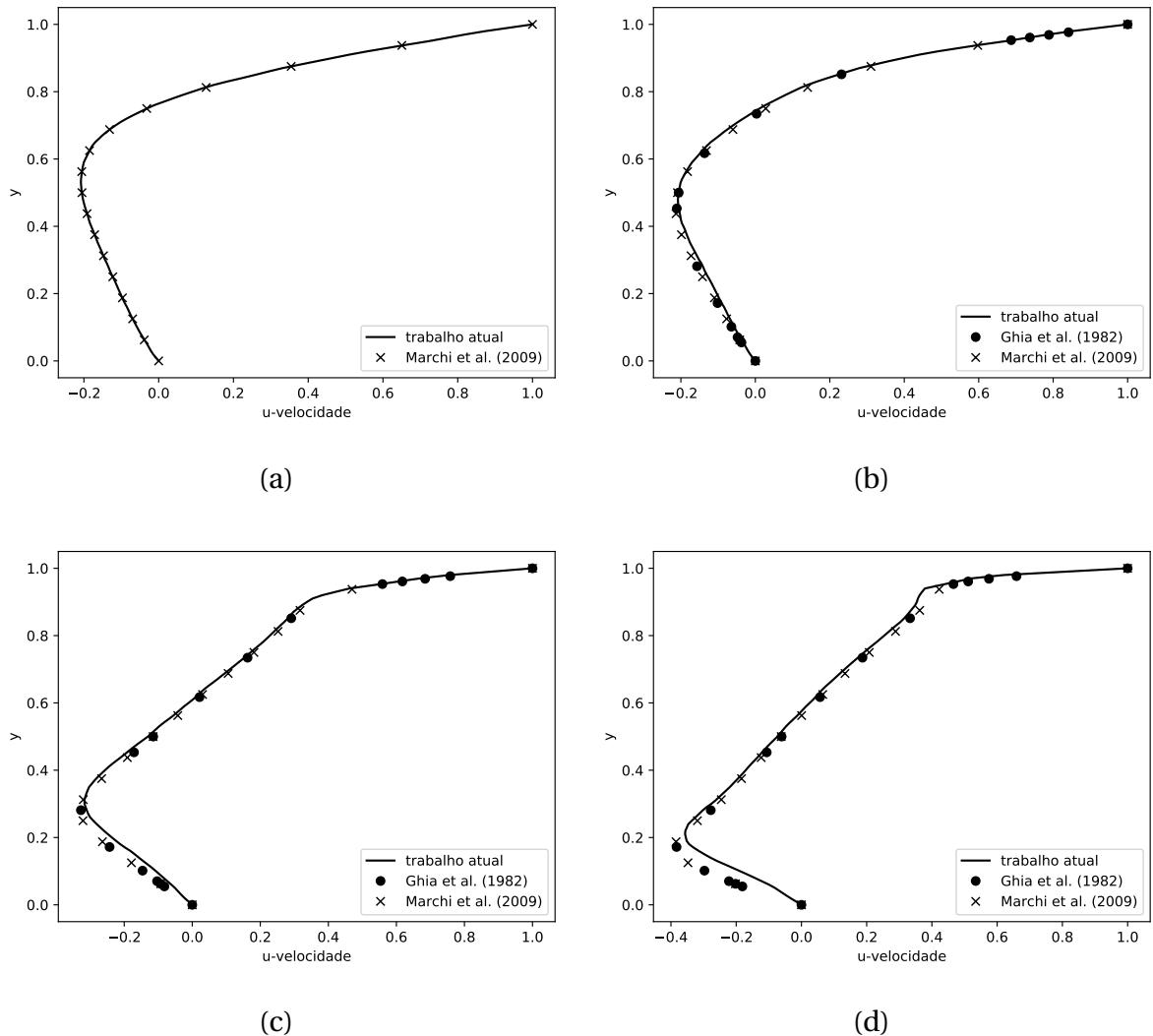


Figure 19: Perfil de u na linha central da cavidade ($x = 0.5$) com diferentes Reynolds: (a) 10 (b) 100 (c) 400 (d) 1000.

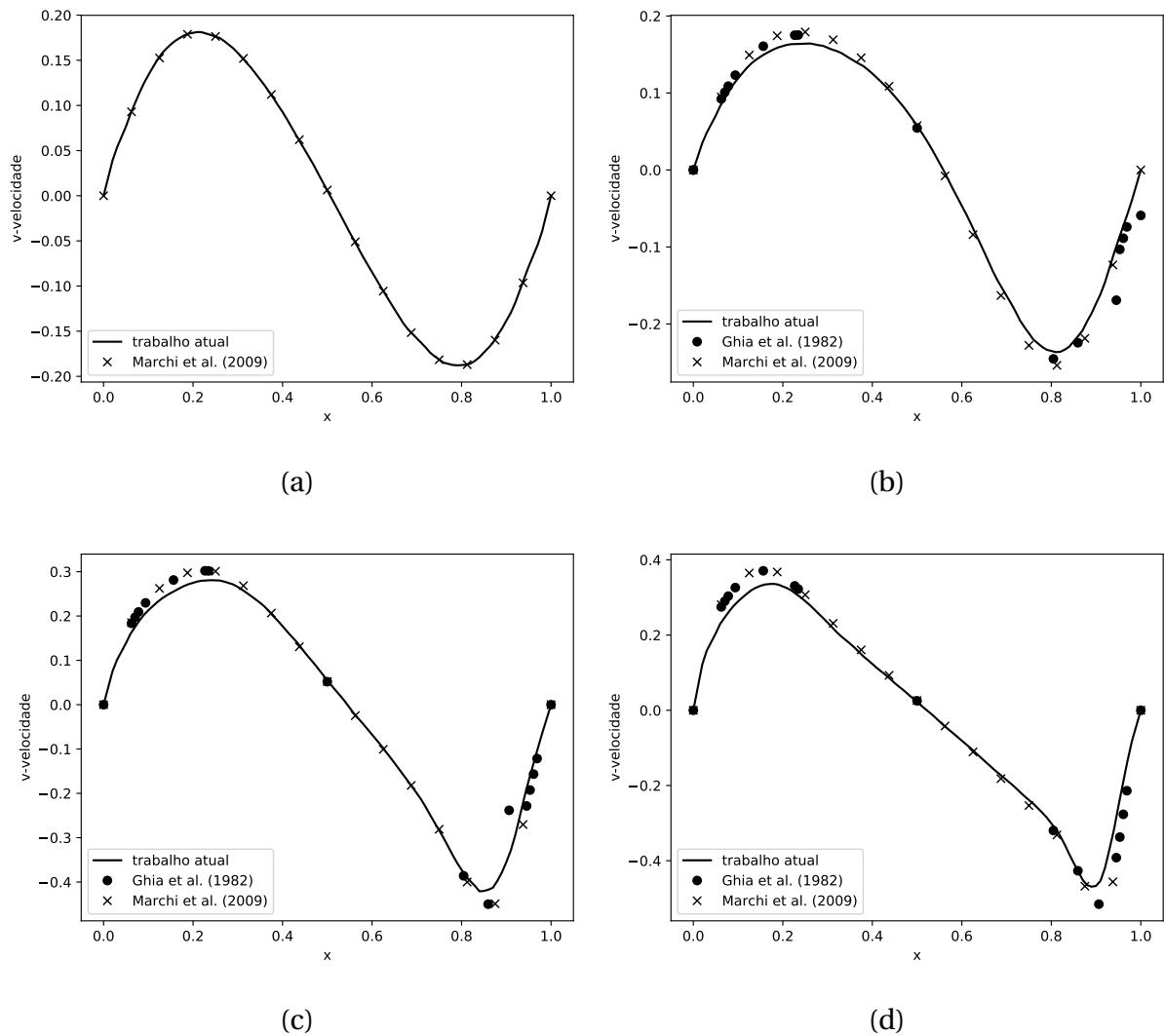


Figure 20: Perfil de v na linha central da cavidade ($y = 0.5$) com diferentes Reynolds: (a) 10 (b) 100 (c) 400 (d) 1000.

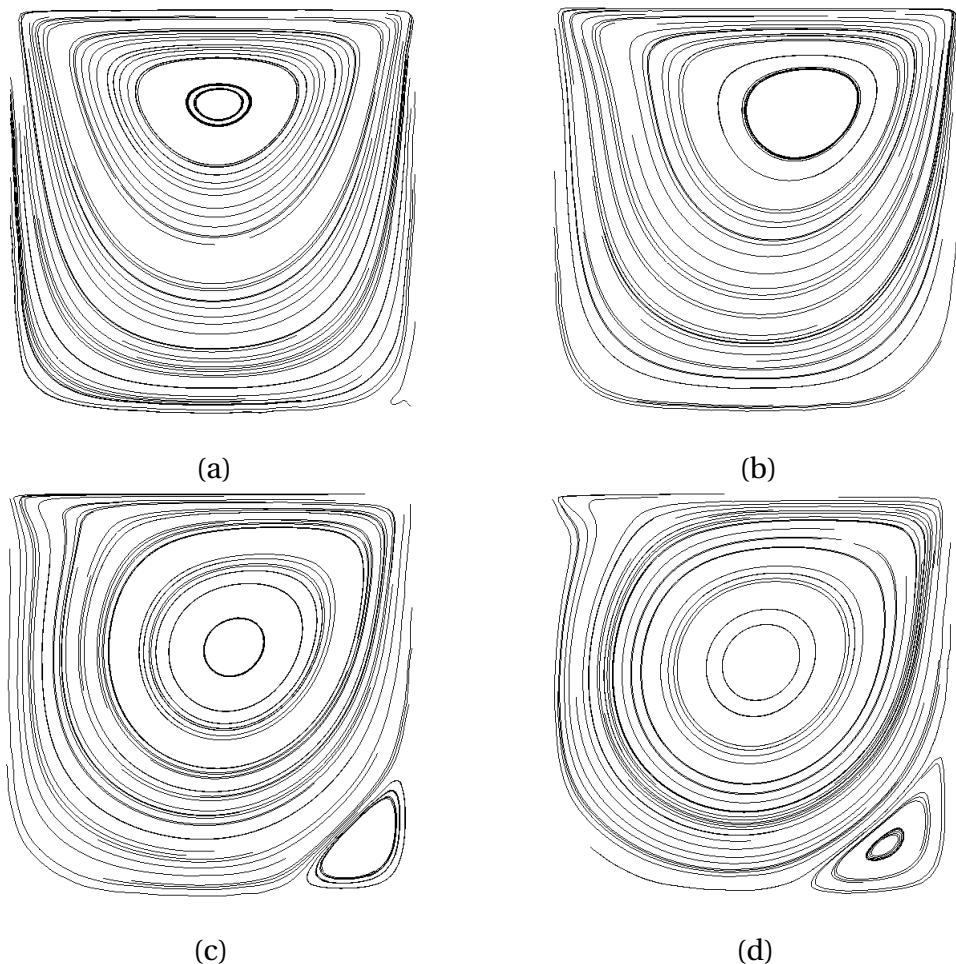


Figure 21: Os contornos da função de corrente para os Reynolds: (a) 10 (b) 100 (c) 400 (d) 1000.

5.6 Escoamento Puramente Convectivo

O transporte de um escalar segundo uma função parabólica e submetido a um escoamento monofásico de um fluido newtoniano e incompressível com elevado número de *Reynold* ($Re \rightarrow \infty$) é conhecido como um *Escoamento Puramente Convectivo*. Neste tipo de escoamento, espera-se que não ocorra difusão do escalar. Para os métodos de aproximação como *MEF* e *MDF*, é possível observar a presença de oscilações espúrias. Como mencionado anteriormente, diversos esquemas podem ser utilizados para reduzir essas oscilações. Apresentaremos nesta seção a utilização do esquema de *Taylor-Galerkin* na redução das oscilações espúrias em comparação ao esquema *Galerkin*. A Figure 22 apresenta esquematicamente o problema e a dinâmica do transporte do escalar.

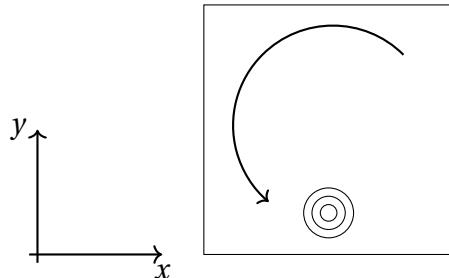


Figure 22: Transporte de um escalar num Escoamento Puramente Convectivo

O domínio foi discretizado utilizando uma malha triangular linear com 1231 nós e 2340 elementos. A equação que governa o escoamento puramente convectivo de um escalar qualquer c é definida como:

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = 0 \quad (5.5)$$

onde $\mathbf{v} = (u, v)$ é o vetor velocidade e suas componentes são definidas como: $u = -y$ e $v = x$. Portanto, espera-se que dado um campo escalar inicial, o mesmo seja deslocado pelo campo de velocidade sem que ocorra difusão, isto é, seu perfil não deve ser alterado enquanto o escoamento acontece. Qualquer alteração no perfil do campo escalar é considerado como erro numérico.

As condições de contorno e inicial utilizadas foram:

- *condição de contorno*: o campo escalar c é especificado com o valor $c = 0$ no contorno da geometria.
- *condição inicial*: o campo escalar é definido segundo a função parabólica $c = 1 - x^2 - y^2$.

A Figure 23 apresenta a comparação do perfil do campo escalar c para os esquemas Galerkin e Taylor-Galerkin em diferentes posições no eixo de rotação conforme o escoamento ocorre. É possível observar que em ambos os esquemas é apresentado oscilações espúrias. No esquema Taylor-Galerkin, porém, tais oscilações são amortecidas diferentemente do esquema Galerkin onde podemos observar que as oscilações espúrias aumentam e o perfil do campo escalar torna-se completamente distorcido.

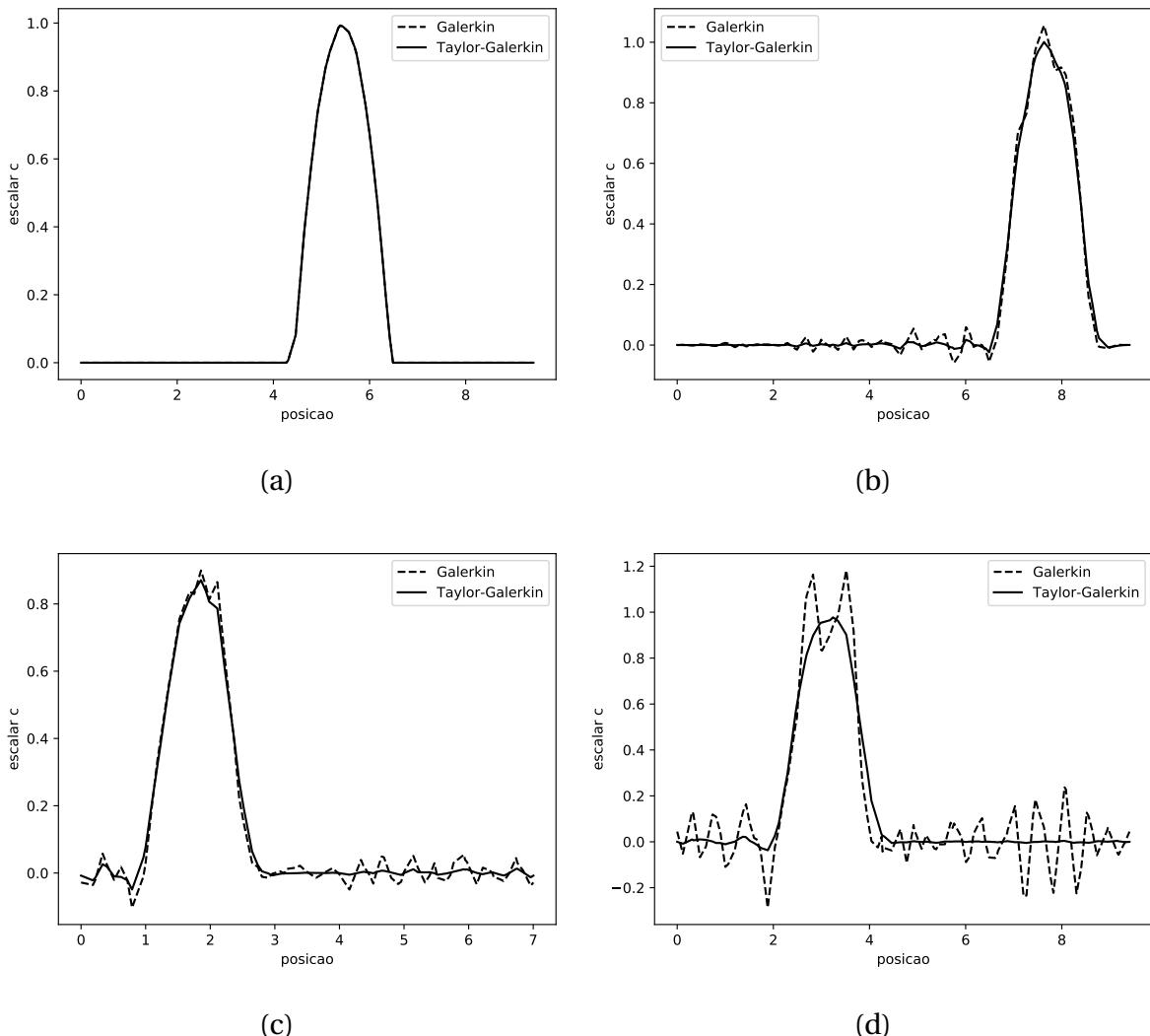


Figure 23: Comparação do perfil de c para os esquemas Galerkin e Taylor-Galerkin em diferentes posições do eixo de rotação: (a) ponto inicial, (b) 1/4 da rotação, (c) 1/2 da rotação e (d) 3/4 da rotação.

As Figure 24 e Figure 25 apresentam a disposição espacial das oscilações espúrias para os esquemas Galerkin e Taylor-Galerkin respectivamente. Como mencionado anteriormente, as oscilações apresentadas no esquema Galerkin distorcem completamente o campo escalar c enquanto no esquema Taylor-Galerkin as mesmas são amortecidas como esperado. Portanto, para os problemas onde as oscilações espúrias estão presentes, o esquema Taylor-Galerkin é superior ao esquema Galerkin.

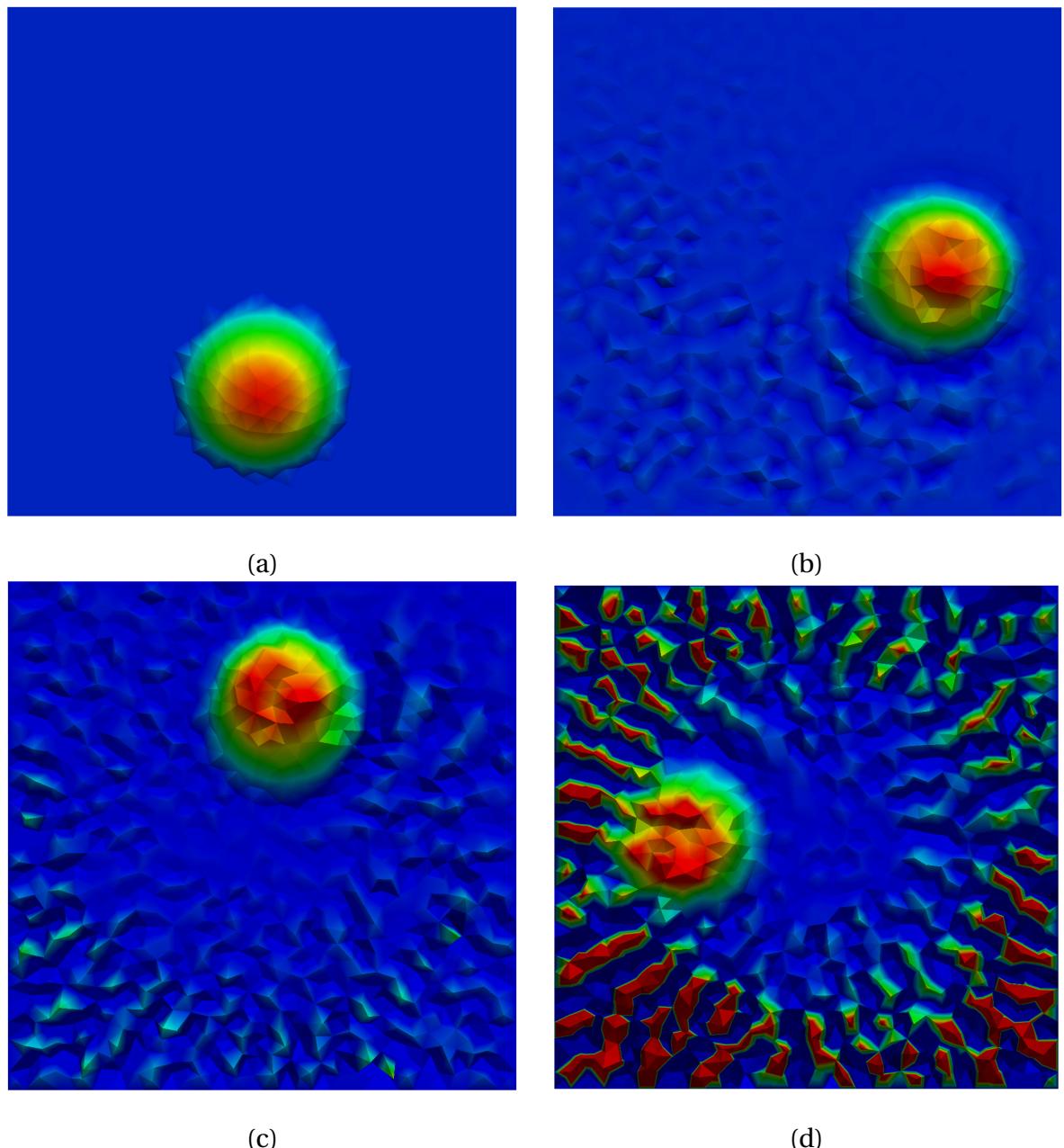


Figure 24: Oscilações espúrias para o esquema Galerkin em diferentes posições do eixo de rotação: (a) ponto inicial, (b) 1/4 da rotação, (c) 1/2 da rotação e (d) 3/4 da rotação.

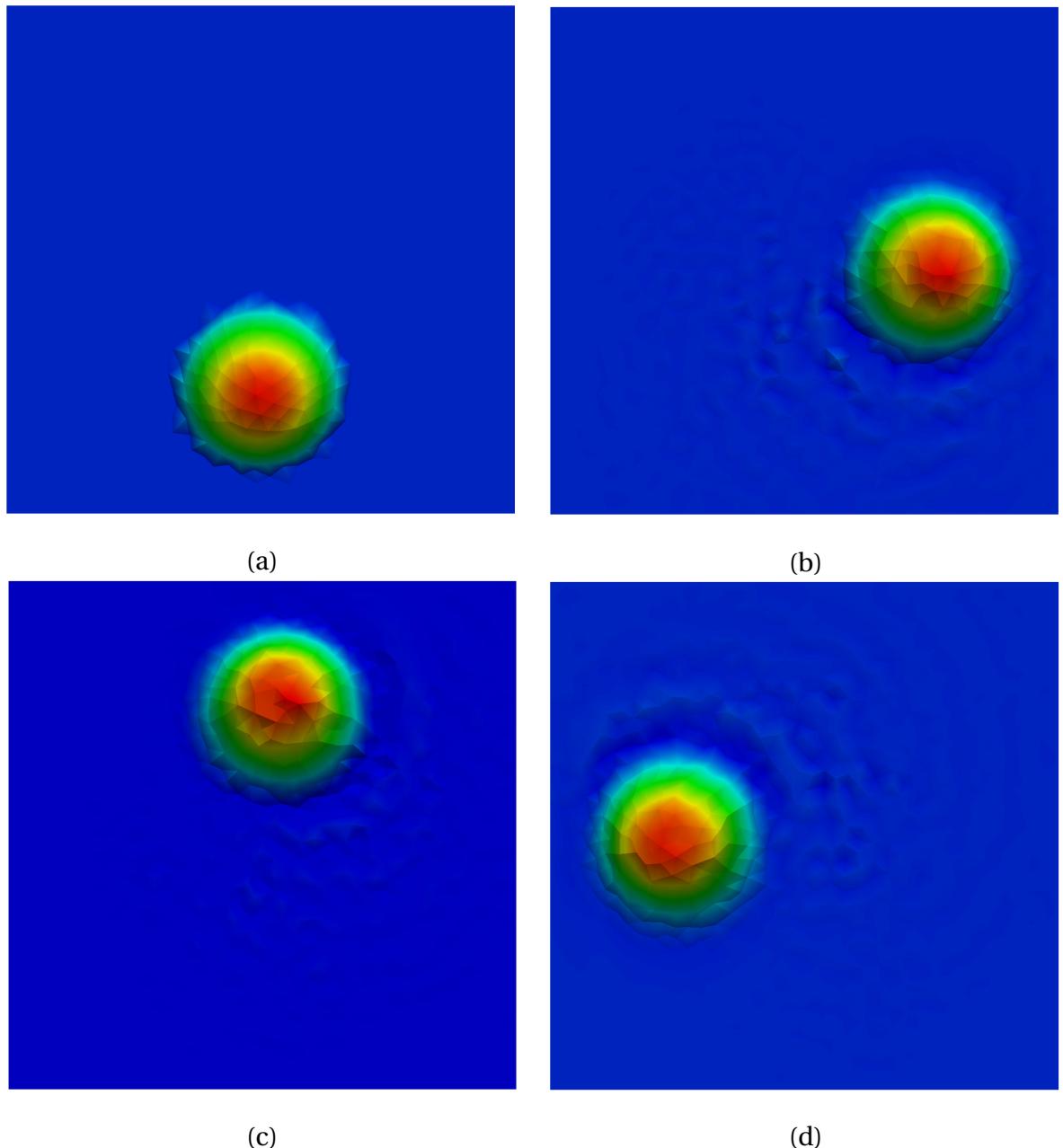


Figure 25: Oscilações espúrias para o esquema Taylor-Galerkin em diferentes posições do eixo de rotação: (a) ponto inicial, (b) 1/4 da rotação, (c) 1/2 da rotação e (d) 3/4 da rotação.

6 RESULTADOS

6.1 Introdução

Neste capítulo são apresentados os resultados da simulações numéricas para o escoamento sanguíneo em uma artéria coronária. O raio do lúmen da artéria coronariana é $R = 0.0015m$, a viscosidade é $\mu = 0.0035Pa.s$ e a massa específica é $\rho = 1060kg/m^3$ como sugerido por Bozsak, Chomaz e Barakat (2014) [16]. De acordo com Kessler et al. (1998) [46], a velocidade do sangue na artéria coronária é $u = 12cm/s$. Dessa forma, o número de Reynolds utilizado será $Re = 54.5$.

A equação de Navier-Stokes é utilizada segundo a formulação corrente-vorticidade com o acoplamento da equação de transporte de espécie química para quatro geometrias propostas por Wang et al. (2017) [9], porém modificadas para coordenadas cartesianas como apresentado na Figure 26. Na seção 6.2, a artéria coronária com aterosclerose é modelada como um escoamento em um canal curvado. Na seção 6.3, é apresentado a simulação para a artéria coronária com aterosclerose e com stent farmacológico colocado para diversos *Schmidt*, tais como $Sc = 1$ e 10 . Na seção 6.4, é apresentado a simulação de uma artéria coronária real com aterosclerose e na seção 6.5, a artéria coronária real com aterosclerose e com stent farmacológico é simulado com diversos números de *Schmidt* como no caso da seção 6.3. Devido a simetria, apenas a metade do domínio foi simulado. A visualização da simulação foi feita pelo software livre *Paraview* proposto por Henderson (2007) [10].

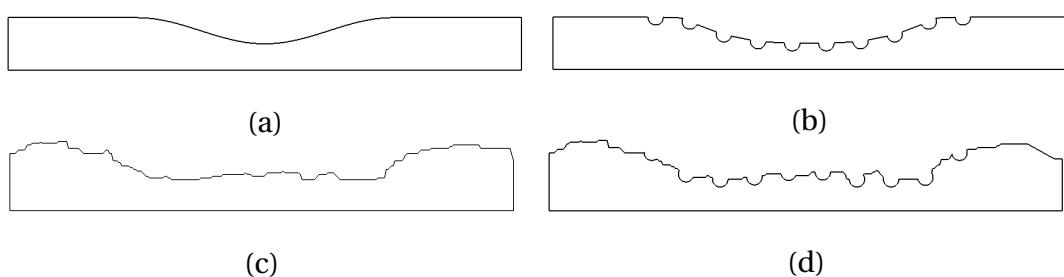


Figure 26: Geometria não dimensional para escoamento sanguíneo em artéria coronária. O raio é $R = 1$ e o comprimento do canal é $L = 10R$. (a) Canal Curvado (b) Canal Curvado com Stent (c) Canal Real e (d) Canal Real com Stent.

As condições de contorno utilizadas nessas simulações foram:

- *condição de entrada:* a componente normal da velocidade é $v = 0$ enquanto a componente tangencial da velocidade é $u = 1$. A função de corrente também é especificada e seu valor é definido segundo a equação da continuidade para um fluido incompressível. Dessa forma, seu valor será $\psi = y$. A derivada da concentração possui o valor nulo $\partial c / \partial n = 0$.
- *condição de não escorregamento:* esta condição é utilizada na parede superior, onde todas as componentes da velocidade são especificadas com os valores $u = 0$ e $v = 0$. A função de corrente também é especificado com o valor de $\psi = 1$. A derivada da concentração possui o valor nulo $\partial c / \partial n = 0$.
- *condição de saída:* O valor da função de corrente é especificado $\psi = y$. As derivadas das componentes tangencial e normal da velocidade e da concentração possuem o valor nulo, isto é, $\partial u / \partial n = 0$, $\partial v / \partial n = 0$ e $\partial c / \partial n = 0$ respectivamente.
- *condição de livre escorregamento:* esta condição é utilizada no eixo de simetria. A componente normal da velocidade e a função de corrente possuem seus valores especificados, tais como $v = 0$ e $\psi = 0$ respectivamente. A derivada da componente tangencial da velocidade e a derivada da concentração possuem também o valor nulo $\partial u / \partial n = 0$ e $\partial c / \partial n = 0$ respectivamente.
- *condição de espécie química:* esta condição é utilizada no stent farmacológico, onde todas as componentes da velocidade são especificadas com os valores $u = 0$ e $v = 0$. A função de corrente e a concentração também são especificados com os valores de $\psi = 1$ e $c = 1$ respectivamente.

Conforme foi informado nas seções anteriores, a condição de contorno do campo de vorticidade é calculado através do algoritmo de solução como apresentado na Figure 10.

6.2 Canal Curvado

Para o caso onde a artéria coronária possui aterosclerose, o problema é modelado como um escoamento entre placas retas e paralelas e curvadas. A geometria utilizada promove uma redução suave da distância entre as paredes superior e inferior do canal. Foi considerado 40% de obstrução do canal devido a aterosclerose e o domínio foi discretizado com 10261 nós e 23049 elementos triangulares lineares.

A Figure 27 apresenta o perfil de velocidade transiente ao longo da coordenada y no meio do canal ($x = 5R$). Como podemos observar, o valor adimensional máximo do campo de velocidade chega a $u = 2.3$ quando a artéria possui aterosclerose, isto é, há um aumento de 53% da velocidade máxima quando comparado com a artéria sem aterosclerose como apresentado na Figure 17.

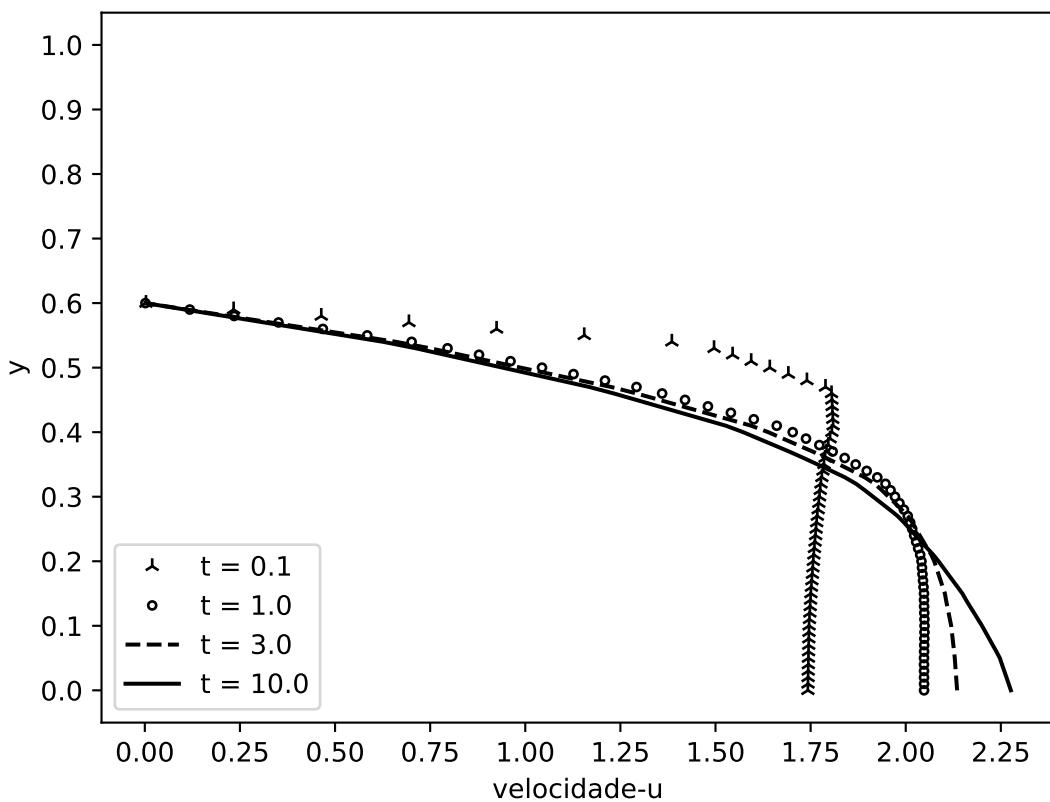


Figure 27: Evolução no tempo do perfil da velocidade para o Canal Curvado.

A Figure 28 apresenta a evolução no tempo e no espaço do campo de velocidade para a metade do domínio, pois os resultados são simétricos na direção y . O campo de velocidade é representado com os valores adimensionais onde a cor vermelha se refere ao valor $u = 2.3$ e a cor azul $u = 0$. Transformando em valores dimensionais temos $u = 27.6\text{cm/s}$ e $u = 0\text{cm/s}$ respectivamente.

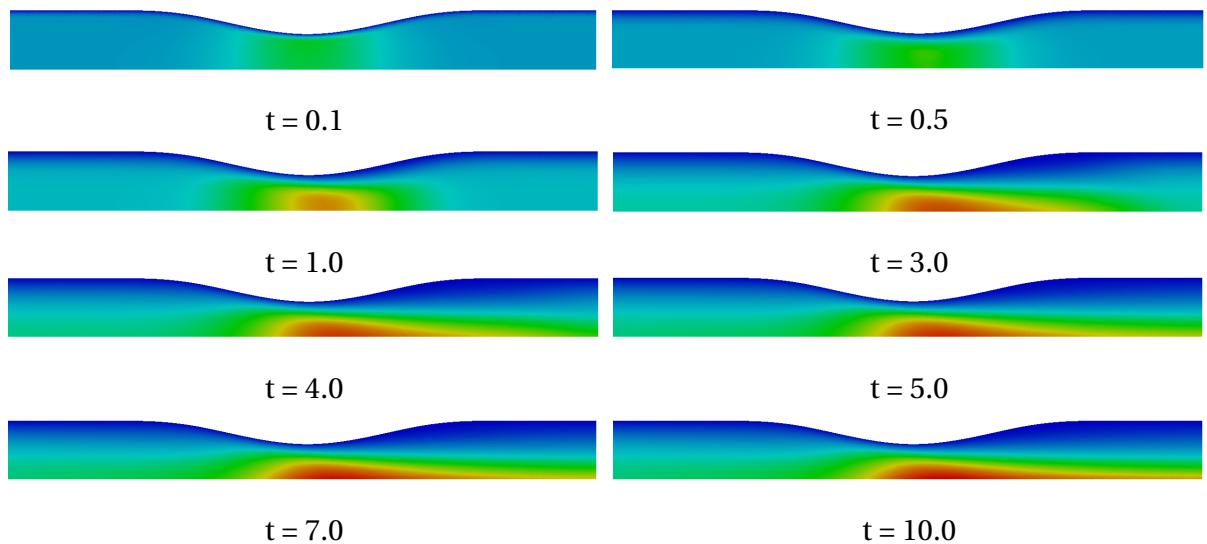


Figure 28: Evolução no tempo e no espaço do campo de velocidade para o Canal Curvado.

6.3 Canal Curvado com Stent Farmacológico

Para este caso, o stent farmacológico é colocado na parte superior do canal curvado. O mesmo é modelado por 10 semi círculos uniformemente espaçados. Assim como no caso anterior, foi considerado uma obstrução de 40% do canal devido a aterosclerose e o domínio foi discretizado com 15875 nós e 35408 elementos triangulares lineares.

A Figure 29 apresenta o perfil de velocidade transiente ao longo da coordenada y no meio do canal ($x = 5R$). Como podemos observar, o valor adimensional máximo do campo de velocidade chega a $u = 3.6$ quando o stent é implantado, isto é, possuímos um aumento de 56% quando comparado com a artéria apenas com aterosclerose como no caso anterior (ver seção 6.2).

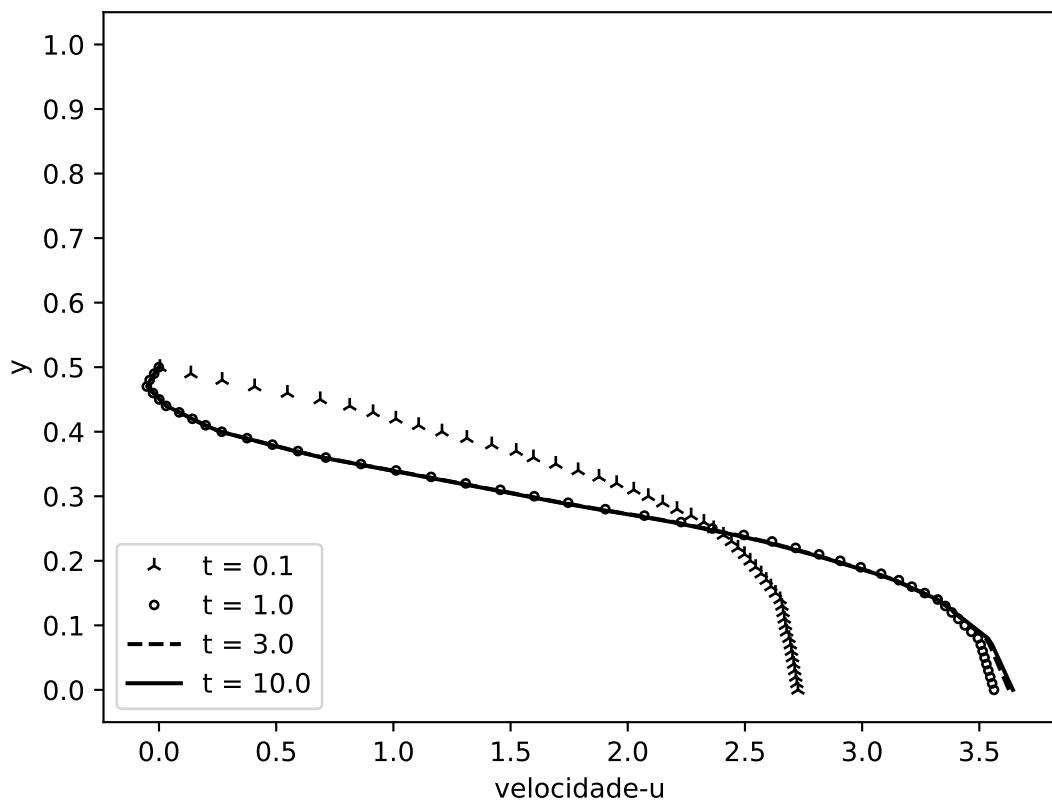


Figure 29: Evolução no tempo do perfil da velocidade para o Canal Curvado com Stent Farmacológico.

A Figure 30 apresenta a evolução no tempo e no espaço do campo de velocidade para a metade do domínio já que os resultados são simétricos na direção y . O campo de velocidade é representado com os valores adimensionais onde a cor vermelha se refere ao valor $u = 3.6$ e a cor azul $u = 0$. Transformando em valores dimensionais temos $u = 43.2\text{cm/s}$ e $u = 0\text{cm/s}$ respectivamente.

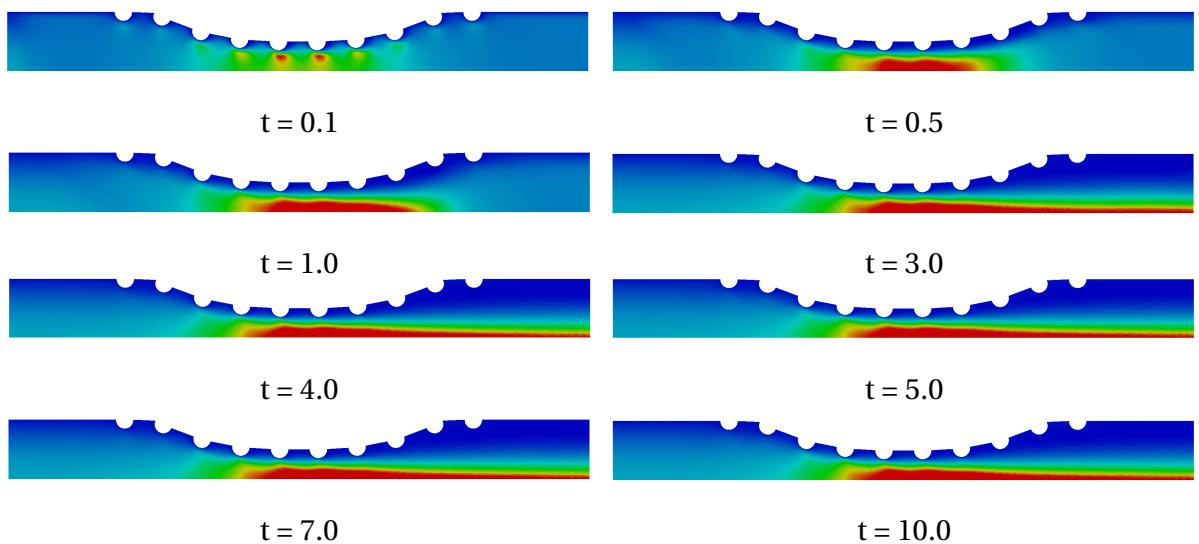


Figure 30: Evolução no tempo e no espaço do campo de velocidade para o Canal Curvado com Stent Farmacológico.

Conforme mencionado por Lucena et al. (2017) [17], é estimado que 47% do fármaco é difundido na corrente sanguínea. A Figure 31 e a Figure 32 apresentam a evolução no tempo e no espaço do campo da concentração para a metade do domínio devido a simetria para diversos números de *Schmidt* tais como: 1 e 10 respectivamente. A concentração é representado com os valores adimensionais onde a cor vermelha representa 100% e a cor azul representa 0% dessa concentração que é difundida na corrente sanguínea. É possível observar que o número de Schmidt influencia diretamente no transporte do fármaco na corrente sanguínea. Para elevados valores do número de *Schmidt*, o transporte de espécie química torna-se puramente convectivo.

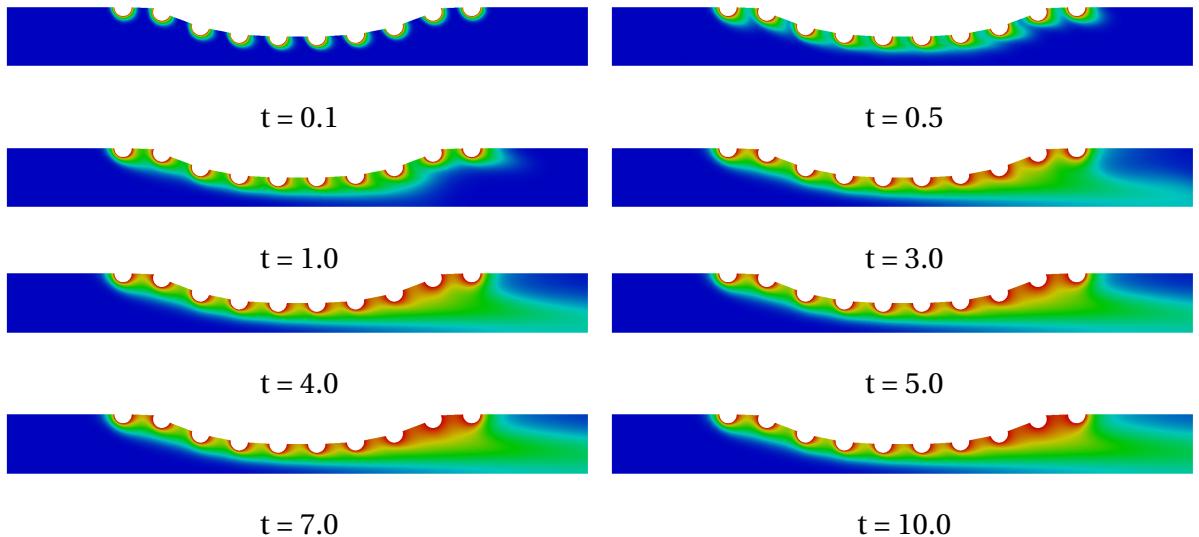


Figure 31: Evolução no tempo e no espaço do campo de espécie química para o Canal Curvado com Stent Farmacológico com $Sc = 1$.

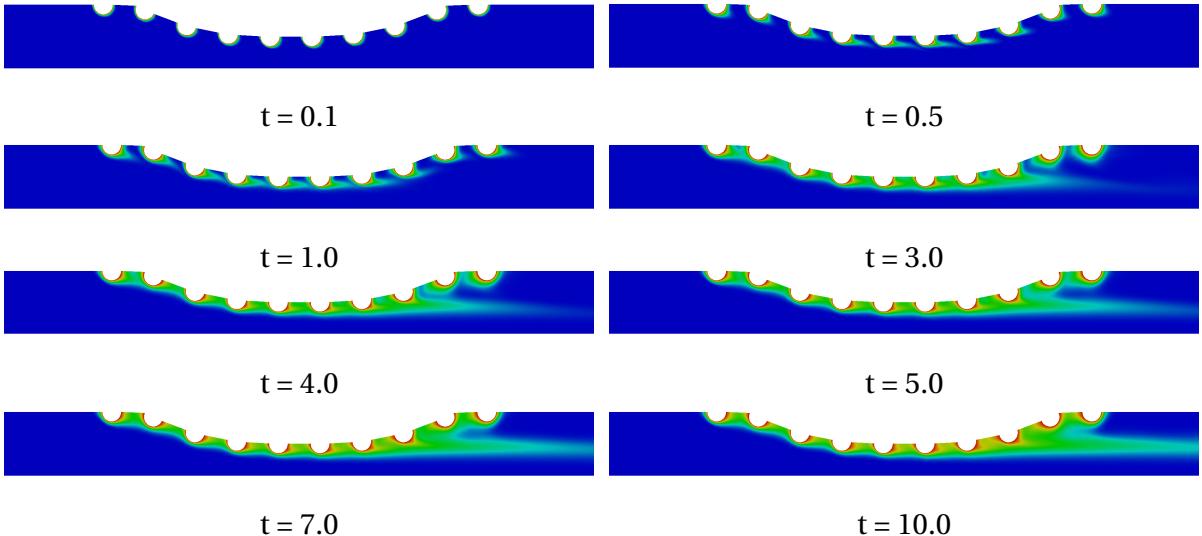


Figure 32: Evolução no tempo e no espaço do campo de espécie química para o Canal Curvado com Stent Farmacológico com $Sc = 10$.

6.4 Canal Real

Para este caso, a simulação numérica é realizada para uma artéria coronária real com aterosclerose cuja geometria foi obtida através de um processamento de imagem como sugerido por Wang et al. (2017) [9]. Essa geometria é particular para cada paciente devido as condições de saúde do mesmo. Assim como nos casos anteriores, foi considerado uma

obstrução de 40% do canal devido a aterosclerose e o domínio foi discretizado com 7632 nós e 14665 elementos triangulares lineares.

A Figure 33 apresenta o perfil de velocidade transiente ao longo da coordenada y no meio do canal ($x = 5R$). O valor adimensional máximo do campo de velocidade chega a $u = 2.25$. Dessa forma, a geometria curvada representa uma boa aproximação como observado na Figure 27.

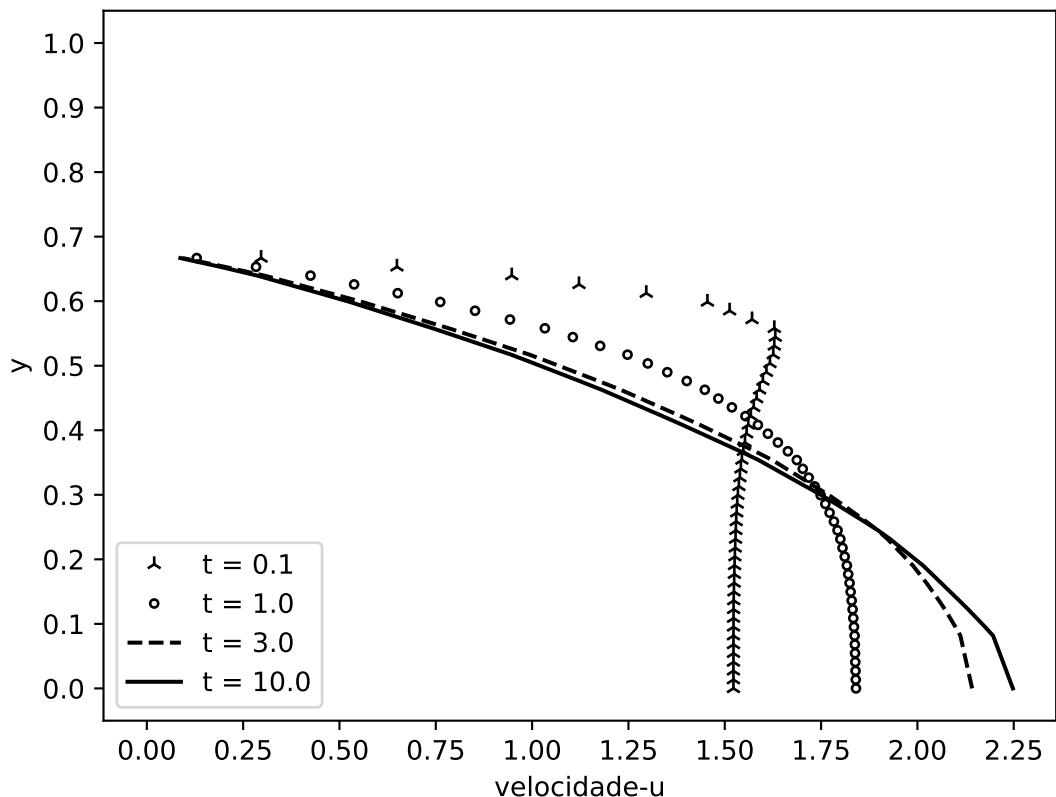


Figure 33: Evolução no tempo do perfil da velocidade para o Canal Real.

A Figure 34 apresenta a evolução no tempo e no espaço do campo de velocidade para a metade do domínio já que os resultados são simétricos na direção y . O campo de velocidade é representado com os valores adimensionais onde a cor vermelha se refere ao valor $u = 2.25$ e a cor azul $u = 0$.

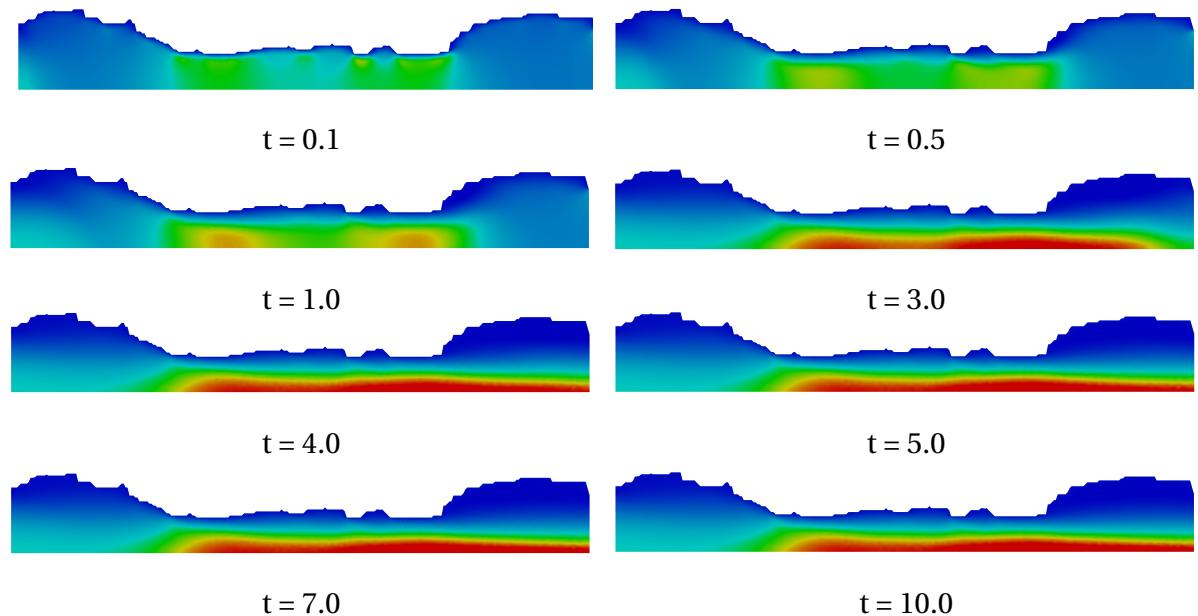


Figure 34: Evolução no tempo e no espaço do campo de velocidade para o Canal Real.

6.5 Canal Real com Stent Farmacológico

Para este caso, o stent farmacológico é colocado na parte superior da artéria coronária real. O mesmo é modelado por 10 semi círculos uniformemente espaçado. Assim como no caso anterior, foi considerado uma obstrução de 40% do canal devido a aterosclerose e o domínio foi discretizado com 11807 nós e 26426 elementos triangulares lineares.

A Figure 35 apresenta o perfil de velocidade transiente ao longo da coordenada y no meio do canal ($x = 5R$). Como podemos observar, o valor adimensional máximo do campo de velocidade chega a $u = 2.65$ quando o stent é implantado, isto é, possuímos um aumento de apenas 18% quando comparado com a artéria sem o stent implantado como no caso anterior. Porém, esse aumento de velocidade pode variar de acordo com o perfil da geometria da artéria coronária para cada paciente.

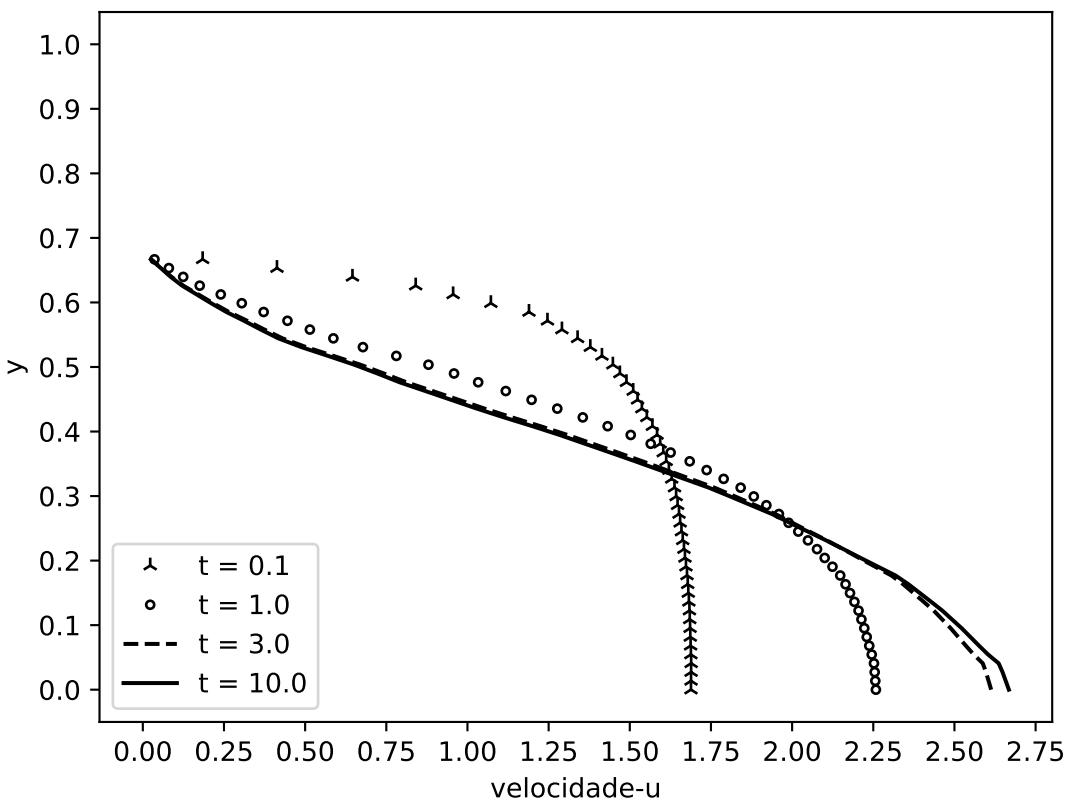


Figure 35: Evolução no tempo do perfil da velocidade para o Canal Real com Stent Farmacológico.

A Figure 36 apresenta a evolução no tempo e no espaço do campo de velocidade para a metade do domínio, pois os resultados são simétricos na direção y . O campo de velocidade é representado com os valores adimensionais onde a cor vermelha se refere ao valor $u = 2.65$ e a cor azul $u = 0$.

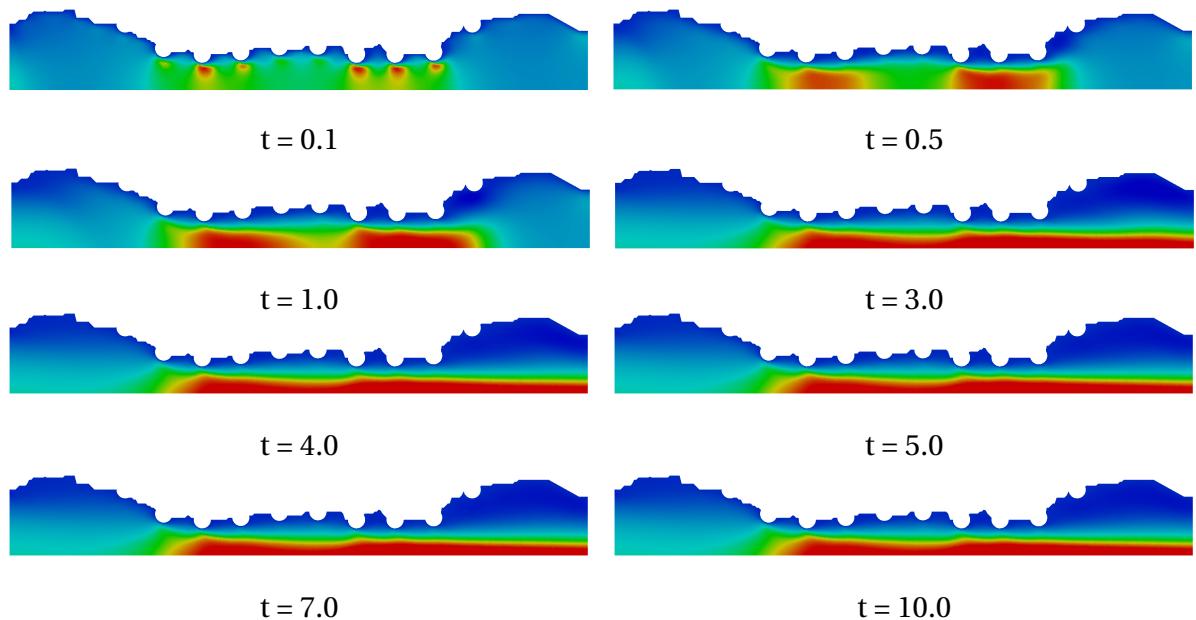


Figure 36: Evolução no tempo e no espaço do campo de velocidade para o Canal Real com Stent Farmacológico.

A Figure 37 e a Figure 38 apresentam a evolução no tempo e no espaço do campo de concentração para a metade do domínio devido a simetria para diversos números de *Schmidt* tais como: 1 e 10, respectivamente. É possível observar a influência do aumento do número de *Schmidt* na difusão do fármaco. A concentração é representada com os valores adimensionais onde a cor vermelha representa 100% e a cor azul representa 0% da concentração que é difundida na corrente sanguínea.

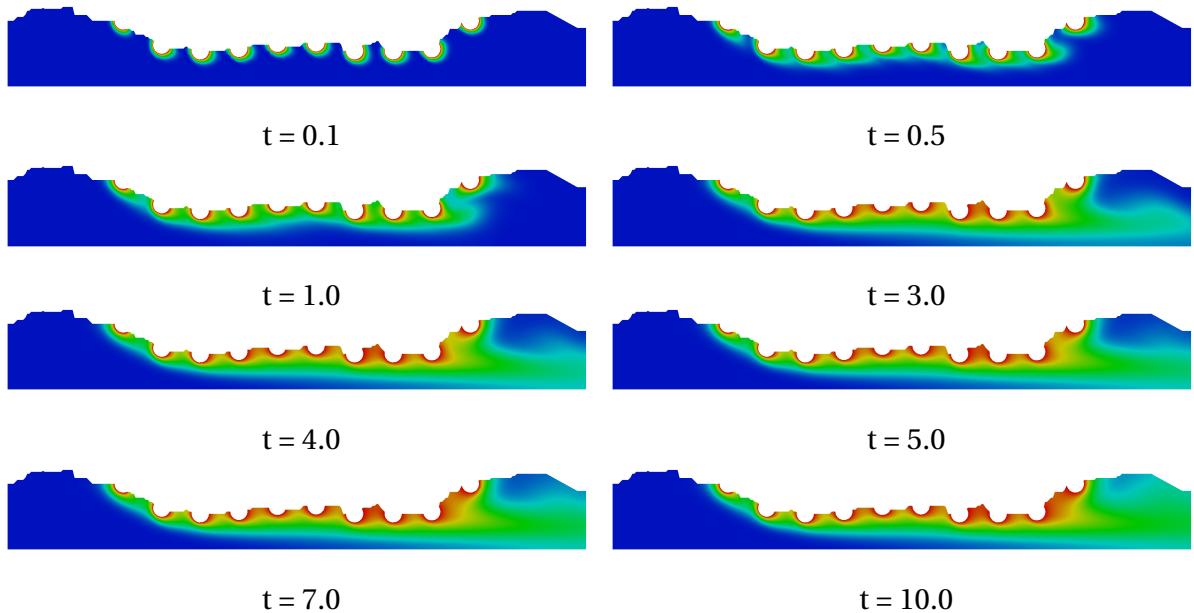


Figure 37: Evolução no tempo e no espaço do campo de espécie química para o Canal Real com Stent Farmacológico com $Sc = 1$.

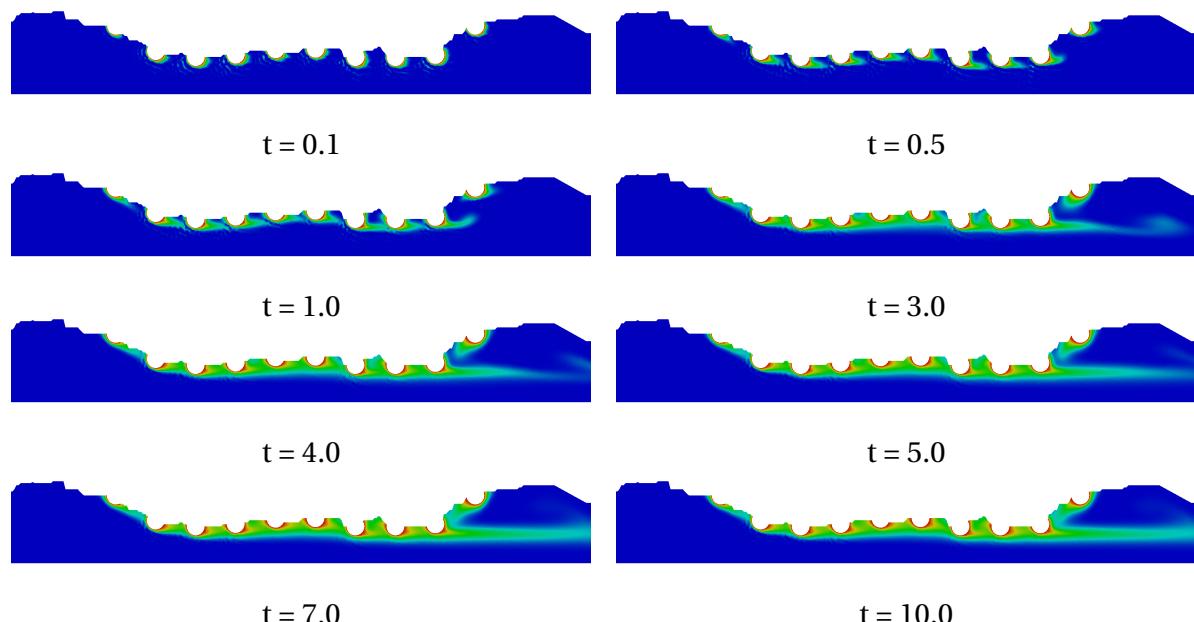


Figure 38: Evolução no tempo e no espaço do campo de espécie química para o Canal Real com Stent Farmacológico com $Sc = 10$.

CONCLUSÃO

Neste trabalho foi apresentado a equação de Navier-Stokes utilizando a formulação corrente-vorticidade com a equação de transporte de espécie química em uma abordagem do Método dos Elementos Finitos em que o esquema Taylor-Galerkin foi aplicado às equações de governo. Como a formulação corrente-vorticidade não apresenta o acoplamento entre a velocidade e pressão, podemos utilizar o elemento triangular linear sem restrição possibilitando assim uma facilidade na implementação do código numérico além das variáveis envolvidas serem escalares e não vetoriais como no caso das variáveis primitivas.

Foi construído um código completo em linguagem de programação de alto nível usando o paradigma de orientação de objetos e a partir do presente momento, possuímos uma plataforma de estudos de problemas de escoamento de fármacos em artérias. O simulador é capaz também de descrever em detalhes problemas envolvendo escoamento de fluidos newtonianos com transporte de natureza escalar (como na concentração e na temperatura) devido a construção generalizada do código.

O código numérico apresentou resultados satisfatórios comparados às soluções analíticas dos *Escoamento de Couette*, *Escoamento de Poiseuille* e *Escoamento de Poiseuille em Meio Domínio* onde a condição de superfície livre escorregamento no eixo de simetria foi aplicada. Foi simulado, também, o escoamento em uma cavidade com tampa móvel (*lid-driven cavity flow*) onde os resultados foram comparados com aqueles apresentados por Ghia et al. (1982) [7] e Marchi et al. (2009) [8] para vários números de Reynolds. Por fim, foi apresentado a comparação entre os esquemas *Galerkin* e *Taylor-Galerkin* para um escoamento puramente convectivo de uma função parabólica onde foi possível observar a eficácia do esquema *Taylor-Galerkin* em comparação ao esquema *Galerkin* para a redução das oscilações espúrias. Dessa forma, a validação do código numérico foi realizada para problemas convectivos-difusivos bidimensionais em coordenadas cartesianas e submetido à condição de contorno de *Dirichlet*.

O objetivo desse trabalho era conhecer a dinâmica do escoamento sanguíneo em uma artéria coronária com aterosclerose e com stent farmacológico implantado. Dessa forma, foi apresentado a simulação para quatro geometrias modeladas como bidimensionais e em coordenadas cartesianas. Foi apresentado o perfil do campo de velocidade para as quatro geometrias propostas onde foi possível observar o aumento da velocidade máxima quando o

stent farmacológico estava implantado. A simulação foi feita utilizando diversos números de *Schmidt*, tais como $Sc = 1$ e 10 . Foi possível verificar na simulação que o número de *Schmidt* influencia diretamente no transporte do fármaco na corrente sanguínea. Para elevados valores do número de *Schmidt*, o transporte de espécie química torna-se puramente convectivo e sua influência na parede da artéria deve ser verificada.

Para trabalhos futuros, destacamos quatro desenvolvimentos:

- Utilização do esquema *Semi-Lagrangeano* para as derivadas materiais em substituição do esquema *Taylor-Galerkin* para a redução das oscilações espúrias
- Utilização das variáveis primitivas na equação de Navier-Stokes em uma abordagem 3D
- Modelar o escoamento sanguíneo como um problema multifásico
- Simular a transferência de espécie química na parede da artéria acoplado ao escoamento no lúmen.

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APÊNDICE - PUBLICAÇÕES

Durante a execução deste estudo, alguns trabalhos foram publicados ou aceitos na forma de artigos em congressos. Este apêndice traz três desses trabalhos. Inicialmente é apresentado o trabalho aceito para publicação pelo *17th Brazilian Congress of Thermal Sciences and Engineering (ENCIT)* que acontecerá em Novembro de 2018. Em seguida, apresentamos o trabalho publicado pelo *X Congresso Nacional de Engenharia Mecânica (CONEM)* com identificação doi://10.26678/ABCM.CONEM2018.CON18-1227 que ocorreu em Maio de 2018. Por fim, é apresentado o trabalho publicado pelo *II Congresso Brasileiro de Fluidodinâmica Computacional (CBCFD)* que ocorreu em Junho de 2018. Abaixo segue um pequeno resumo desses trabalhos:

BLOOD FLOW DYNAMICS SIMULATION IN CORONARY ARTERY WITH DRUG-ELUTING STENT USING FINITE ELEMENT METHOD

17th Brazilian Congress of Thermal Sciences and Engineering (ENCIT 2018)

Novembro/2018 - Aceito para a publicação

The present work aims at developing a computational framework to simulate coronary artery flows in cartesian coordinates. The Finite Element Method (FEM) is used to solve the governing equations of the blood flow in coronary artery with drug-eluting stent placed. The blood was modeled as single-phase, incompressible and newtonian fluid. The Navier-Stokes equation is shown according to the stream-vorticity formulation with coupled species transport equation. The Taylor-Galerkin scheme were used to decrease spurious oscillations as seen for moderate to high Reynolds number. The code proved to be effective by results presented in validation cases. The dynamics of blood flow was shown to a coronary artery with atherosclerosis and drug-eluting stent placed. Therefore, the streamfunction and vorticity formulation showed an useful approximation for to calculate the velocity and concentration fields since the variables are scalars allowing then a smooth implementation.

A NUMERICAL SIMULATION OF BLOOD FLOW DYNAMICS IN CORONARY ARTERY USING STREAMFUNCTION-VORTICITY FORMULATION

X Congresso Nacional de Engenharia Mecânica (CONEM 2018)

Maio/2018 - Publicado

doi://10.26678/ABCM.CONEM2018.CON18-1227

The present work aims at developing a computational framework to simulate coronary artery flows in cartesian coordinates. An accurate method capable of capturing the flow dynamics is strictly required. In this paper a Finite Element Method (FEM) is used to solve the governing equations of the motion of the blood flow found in coronary artery as incompressible fluid using the stream-vorticity formulation with coupled mass transport. The validation of the numerical solution was done by well-known benchmark lid-driven cavity problem and the results were compared with others authors as well as the Hagen-Poiseuille flow for the case straight channel that was compared with analytical solution. The streamfunction and vorticity formulation showed an useful approximation for to calculate the velocity and concentration fields since the variables are scalars allowing then a smooth implementation.

BLOOD FLOW SIMULATION USING STREAM FUNCTION-VORTICITY FEM FORMULATION

II Congresso Brasileiro de Fluidodinâmica Computacional (CBCFD 2018)

Junho/2018 - Publicado

The present work aims at developing a computational framework to simulate coronary artery flows in cartesian coordinates. An accurate method capable of capturing the flow dynamics is strictly required. In this paper a Finite Element Method (FEM) is used to solve the governing equations of the motion of the blood flow found in coronary artery as incompressible fluid using the stream-vorticity formulation with coupled species transport equation. The results were shown for two-dimensional domain in complex geometries of modeled coronary artery channel. The numerical simulation was performed using the streamfunction and vorticity formulation with coupled species transport equation by finite element method approach. The streamfunction and vorticity formulation showed a smooth implementation for to calculate the variables since they are scalars. However, there is a significant difference between the results shown in cartesian coordinates and those shown by Wang et al. (2017) in axisymmetric coordinates.

ENCIT-2018-0357

BLOOD FLOW DYNAMICS SIMULATION IN CORONARY ARTERY WITH DRUG-ELUTING STENT USING FINITE ELEMENT METHOD

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Abstract: The present work aims at developing a computational framework to simulate coronary artery flows in cartesian coordinates. The Finite Element Method (FEM) is used to solve the governing equations of the blood flow in coronary artery with drug-eluting stent placed. The blood was modeled as single-phase, incompressible and newtonian fluid. The Navier-Stokes equation is shown according to the stream-vorticity formulation with coupled species transport equation. The Taylor-Galerkin scheme were used to decrease spurious oscillations as seen for moderate to high Reynolds number.

Keywords: Stream-Vorticity Function, Finite Element Method, Taylor-Galerkin Method, Drug-Eluting Stent, Hemodynamics.

1. INTRODUCTION

According to the World Health Organization (2017), more people die annually from the cardiovascular diseases (CVDs) than from any other cause in the world. An estimated 17.7 million people died from CVDs in 2015, representing 31% of all global deaths. About 41% of these deaths were due to coronary artery disease (CAD). The leading cause of the CAD is atherosclerosis where the diameter of the vessel is decreased. Two treatments can be performed: coronary artery bypass grafting (CABG) or percutaneous transluminal coronary angioplasty (PTCA). The PTCA is a minimally invasive procedure where a small wire tube, called stents, is placed. This work aims to develop a Finite Element code for stream-vorticity formulation coupled species transport equation and to know how the dynamics of blood flow in coronary artery with atherosclerosis and with stents struts placed.

The dynamics of blood flow in coronary artery and possible influence of stents struts with computational fluid dynamics (CFD) requires a robust numerical method to compute the solution of the differential equations in a relevant model. The equations that govern the dynamics of blood flow in a coronary artery were developed according to continuum media assumption. Thus, the universal conservation laws such as conservation of mass, conservation of momentum and conservation of species transport were used. The blood was modeled as single-phase, incompressible and newtonian fluid, the diffusion coefficient was considered as constant. The Navier-Stokes equation is shown according to the 2D stream-vorticity formulation with coupled species transport equation in a Finite Element Method approach.

The domain was discretized on an unstructured triangular mesh using the *GMSH* open source as proposed by Geuzaine and Remacle (2009). According to decoupling between velocity field and pressure field achieved by stream-vorticity formulation, the linear triangular element was used. The equations were discretized in time by Taylor series expansion remaining the second order terms to decrease spurious oscillations as seen for moderate to high Reynolds number. Then, the Galerkin formulation was used to discretize in space. Therefore, the Taylor-Galerkin scheme was used as proposed by Donea (1984).

The computational development was done in *Python* language using object-oriented programming paradigm with the aim of reusability and further development. The code validation was made by comparison numerical solution and analytical solution of the *Poiseuille* flow. The comparison of velocity field was done for lid-driven cavity flow with those shown by Ghia *et al.* (1982) and Marchi *et al.* (2009). The dynamics of blood flow and species transport in coronary artery was investigated in 2 test cases as suggested by Wang *et al.* (2017), however modified for 2D cartesian coordinates. The simulation was shown using *Paraview* open source as proposed by Henderson (2007).

2. MATHEMATICAL MODEL

A 2-dimensional Finite Element Method approach is employed to analyse the dynamics of blood flow in coronary artery with atherosclerosis and possible influence of stents struts. The governing equations were developed according to continuum media assumption. Thus, the universal conservation laws such as conservation of mass, conservation of momentum and conservation of species transport were used. The blood was modeled as single-phase, incompressible and newtonian fluid, the diffusion coefficient was considered as constant. The Navier-Stokes equation is shown according to stream-vorticity formulation with coupled species transport equation.

$$\frac{\partial \omega}{\partial t} + \mathbf{v} \cdot \nabla \omega = \frac{1}{Re} \nabla^2 \omega \quad (1)$$

$$\nabla^2 \psi = -\omega \quad (2)$$

$$\mathbf{v} = \mathbf{D}\psi \quad (3)$$

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \frac{1}{ReSc} \nabla^2 c \quad (4)$$

Where, ω is the vorticity field, ψ is the stream function field, c is the concentration field, $\mathbf{v} = (u, v)$ is the velocity field, $\mathbf{D} = [\partial/\partial y, -\partial/\partial x]$ is a mathematical operator, $Re = \rho u D / \mu$ is the Reynolds number, $Sc = \nu / D$ is the Schmidt number, x and y are the independent spatial variables and t is the time variable.

2.1 Finite Element Method

The domain was discretized on an unstructured triangular mesh using the *GMSH* open source as proposed by Geuzaine and Remacle (2009). According to decoupling between velocity field and pressure field achieved by stream-vorticity formulation, the use of linear triangular element was used. The equations were discretized in time by Taylor series expansion remaining the second order terms to decrease spurious oscillations as seen for moderate to high Reynolds number. Then, the Galerkin formulation was used to discretize in space. Therefore, the Taylor-Galerkin scheme was used as proposed by Donea (1984). The governing equations in matrix form used in this paper were:

$$\left[\frac{M}{\Delta t} + \frac{1}{Re} [K_{xx} + K_{yy}] \right] \omega^{n+1} = \frac{M}{\Delta t} \omega^n - u \cdot G_x \omega^n - v \cdot G_y \omega^n - u \frac{\Delta t}{2} [u K_{xx} + v K_{yx}] \omega^n - v \frac{\Delta t}{2} [u K_{xy} + v K_{yy}] \omega^n \quad (5)$$

$$[K_{xx} + K_{yy}] \psi = M \omega \quad (6)$$

$$Mu = G_y \psi \quad (7)$$

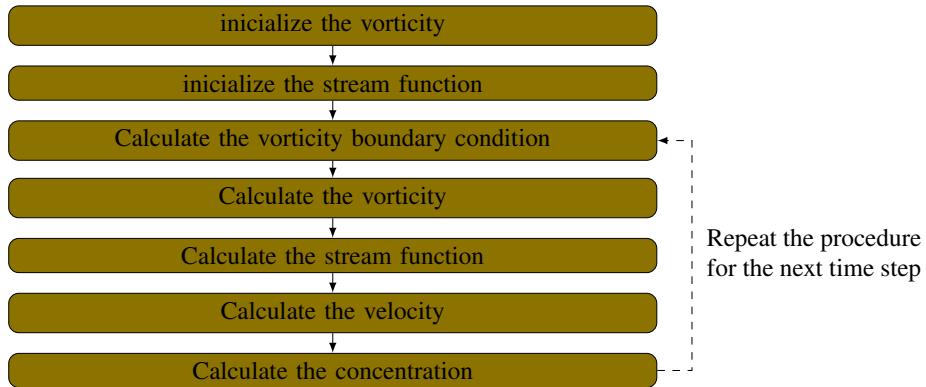
$$Mv = -G_x \psi \quad (8)$$

$$\left[\frac{M}{\Delta t} + \frac{1}{ReSc} [K_{xx} + K_{yy}] \right] c^{n+1} = \frac{M}{\Delta t} c^n - u \cdot G_x c^n - v \cdot G_y c^n - u \frac{\Delta t}{2} [u K_{xx} + v K_{yx}] c^n - v \frac{\Delta t}{2} [u K_{xy} + v K_{yy}] c^n \quad (9)$$

Where, M is mass matrix, G_x and G_y are gradient matrix, K_{xx} , K_{xy} , K_{yx} and K_{yy} are stiffness matrix. The last term of the Eqs. 5 and 9 is known as numerical diffusion and it decrease the spurious oscillations as seen for moderate to high Reynolds numbers. For scalars, *Taylor Galerkin Method* and *Characteristic Galerkin* produce the same result as showed by Lohner *et al.* (1984). The superscripts $n+1$ and n are the scalar that will be calculated and that was calculated in the previous time step, respectively.

2.2 Numerical Solution

The computational development was done in *Python* language using object-oriented programming paradigm with the aim of reusability and further development. The linear system of equations that come from implementing the FEM is solved through iterative method *Conjugate Gradient Solver* available in the public library for scientific tools *SciPy* maintained by Jones *et al.* (2001). The solution algorithm used is shown below:



The first and second steps are out of time loop, while the third to the seventh step are inside of time loop. The application of the boundary condition in the equation can be before loop, except for the vorticity equation (*fourth step*) that the boundary condition must be applied at each time step.

3. VALIDATION

The code validation was made by comparison numerical solution and analytical solution of the *Poiseuille flow*. The comparison of velocity field was done for lid-driven cavity flow with those shown by Ghia *et al.* (1982) and Marchi *et al.* (2009).

3.1 Poiseuille Flow

A single-phase flow, steady and fully developed of an incompressible and newtonian fluid between parallel horizontal plates and stationary is maintained due to a pressure gradient. This flow is known as *Poiseuille flow*. In Fig. ?? is shown a schematic representation of the numerical domain used to simulate the Poiseuille Flow problem, where no-slip condition were used at the top and bottom walls, while an inflow and outflow conditions were set in the plane $x = 0$ and $x = 5L$ respectively.

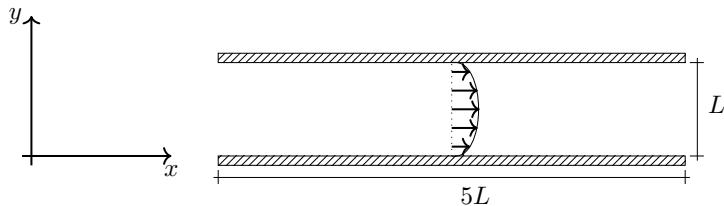


Figure 1: Poiseuille flow

The boundaries conditions used were:

- *inflow condition*: the normal velocity component is set to null value $v = 0$. The tangent velocity component is set to parabolic profile by exact solution, that is, $u = [4u_{max}y/L^2][L - y]$, where $u_{max} = 1.5$. The streamfunction is also specified and its value is defined according to continuity equation for an incompressible fluid. Thus, its value is $\psi = [2u_{max}y^2/3L^2][3L - 2y]$.
 - *No-slip condition*: all the velocity components are specified with null value $u = 0$ and $v = 0$. The streamfunction is also specified $\psi = 1$ in top plate and $\psi = 0$ in bottom plate.

- *outflow condition:* no value is specified. The derivatives of the tangent velocity component, of the normal velocity component and of streamfunction are set to null values, that is, $\partial u/\partial n = 0$, $\partial v/\partial n = 0$ and $\partial \psi/\partial n = 0$ respectively.

The velocity field profile is calculated by equation below:

$$u = \frac{4u_{max}}{L^2}y[L - y] \quad (10)$$

Where, u_{max} is maximum velocity and its value is $u_{max} = 1.5$, L is non-dimensional width between parallel plates and its value is $L = 1$ and y is length between parallel plates and ranges $y = [0, 1]$. The domain was discretized using a linear triangular mesh with 3835 nodes and 7299 elements.

The Fig. 2 shown the evolution of velocity field profile in time when $Re = 100$, the comparasion is also shown between numerical solution and analytical solution. Therefore, the code shown a satisfactory result.

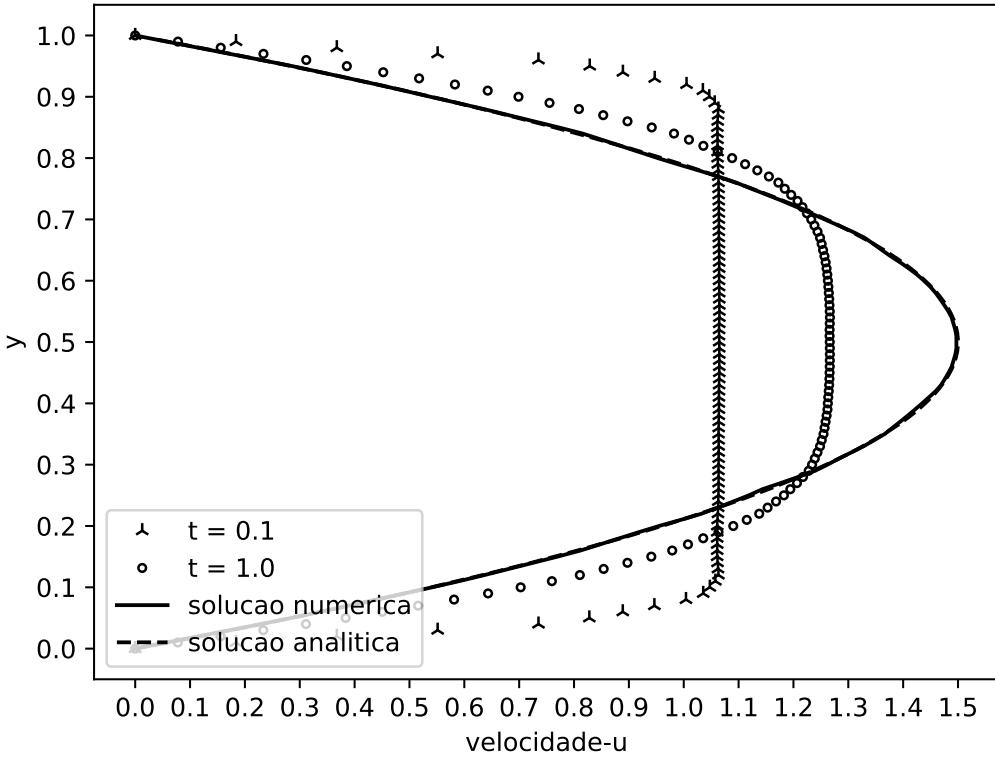


Figure 2: Evolution of velocity field profile in time for $Re = 100$ and the comparison between numerical solution and analytical solution.

3.2 Lid-driven Cavity Flow

A flow on cavity when side and bottom plates are stationary and top plate moves with velocity constant such that $U = top = 1$ is known as *lid-driven cavity flow*. In Fig. ?? is shown a schematic representation of the numerical domain used to simulate the Lid-driven Cavity Flow problem, where no-slip condition were used at the bottom and side walls, while at top wall, the velocity was set $u = U_{top}$.

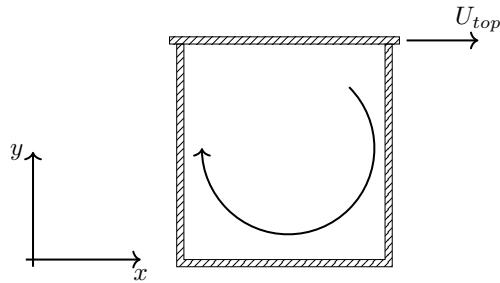


Figure 3: Lid-driven cavity flow

Were simulated flows for the following Reynolds numbers: (Re): 10, 100, 400 and 1000. The dimensions domain in x-direction and y-direction are [0,1]. We used a mesh with 1563 nodes and 2988 elements

The boundaries conditions used were:

- *top plate moves*: all the velocity components are specified with $v = 0$ and $u = U_{top}$, where $U_{top} = 1$. The streamfunction is also specified and its value is $\psi = 0$.
- *No-slip condition*: This condition is used on side and bottom plates. All the velocity components are also specified with null value $u = 0$ and $v = 0$. The streamfunction is specified as $\psi = 0$.

The Figs. 4 and 5 shown profile of u and v components respectively for several Reynolds numbers. The results were compared with Ghia *et al.* (1982) and Marchi *et al.* (2009). Therefore, the code shown a satisfactory result.

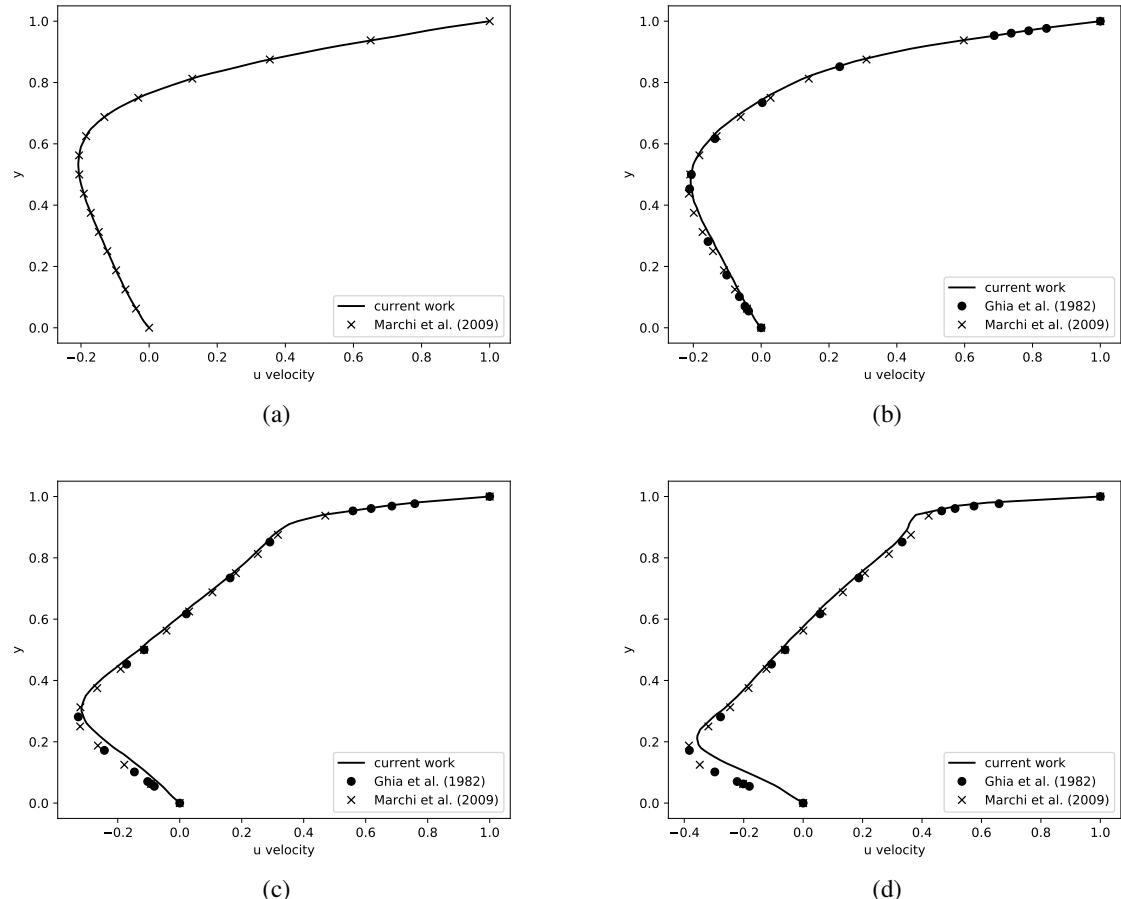


Figure 4: Centerline u velocity profile ($x = 0.5$) in a lid-driven cavity for different Reynolds numbers: (a) 10 (b) 100 (d) 400 (f) 1000.

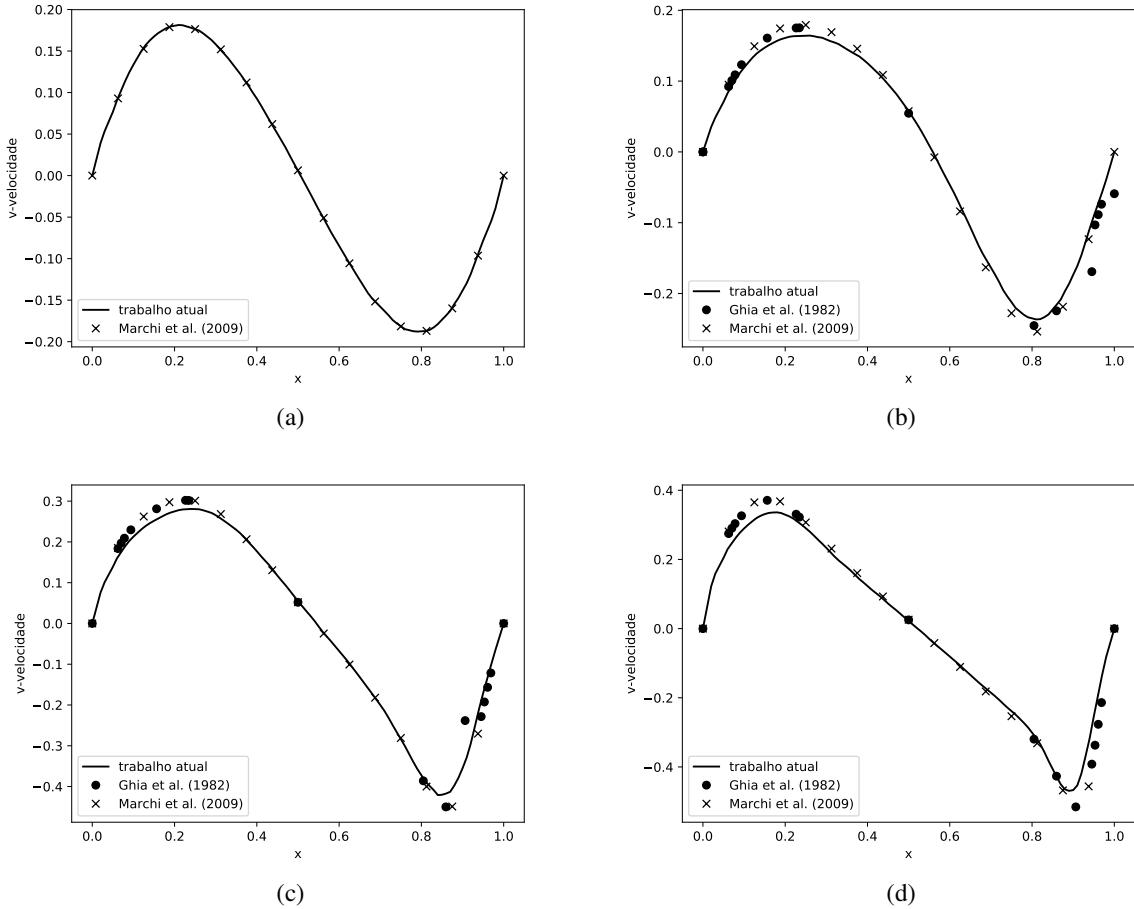


Figure 5: Centerline v velocity profile ($y = 0.5$) in a lid-driven cavity for different Reynolds numbers: (a) 10 (b) 100 (d) 400 (f) 1000.

4. RESULTS AND DISCUSSION

Some results of simulations are shown to demonstrate its capability of using unstructured triangular meshes on various geometries and combination of geometries. Numerical results are given for several cases of blood flows in artery when $Sc = 10$. The post-processing was performed by open source software *PARAVIEW* proposed by Henderson (2007). The lumen radius of a typical artery is about $R = 0.0015\text{m}$, viscosity in the lumen are set to $\mu = 0.0035\text{Pa.s.}$ and density $\rho = 1060\text{kg/m}^3$ as suggested by Bozsak *et al.* (2014). According to Kessler *et al.* (1998), the velocity of the flow at coronary artery is $v = 12\text{cm/s.}$ Therefore, the Reynolds number is $Re = 54.5.$

The Navier-Stokes equation is used according to stream-vorticity formulation with species transport equation coupled for 2 different geometries proposed by Wang *et al.* (2017) and is shown in the Fig. 6, however modified for cartesian coordinates. According to symmetry on y coordinate, half domain was simulated.

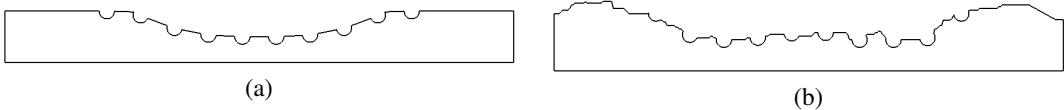


Figure 6: Non-dimensional geometry for blood flow dynamics in coronary arteries. The channel length $L = 10R$ is based on the channel width $R = 1.$ (a) Curved Channel with Stent and (b) Real Channel with Stent.

The boundaries conditions used were:

- *inflow condition:* the normal velocity component is set to null value $v = 0.$ The tangent velocity component is set

to parabolic profile by exact solution, that is, $u = u_{max} [1 - (y/L)^2]$, where $u_{max} = 1.5$. The streamfunction is also specified and its value is defined according to continuity equation for an incompressible fluid. Thus, its value is $\psi = [u_{max}y/3] [3 - (y/L)^2]$.

- *No-slip condition*: this condition is used on bottom plate. all the velocity components are specified with null value $u = 0$ and $v = 0$. The streamfunction is also specified $\psi = 1$ and the derivative of concentration has null value $\partial c/\partial n = 0$.
- *outflow condition*: no value is specified. The derivatives of the tangent velocity component, of the normal velocity component and of streamfunction are set to null values, that is, $\partial u/\partial n = 0$, $\partial v/\partial n = 0$, $\partial \psi/\partial n = 0$ and $\partial c/\partial n = 0$ respectively.
- *Free-slip condition*: used when a symmetry condition is desired. The normal velocity component is set to null value $v = 0$ as well as the streamfunction $\psi = 0$. The derivative of the tangent velocity component and the derivative of the concentration are also set to null value $\partial u/\partial n = 0$ and $\partial c/\partial n = 0$ respectively.
- *Strut condition*: used on the stent. The normal velocity component and the tangent velocity component are specified with null value $u = 0$ and $v = 0$. The streamfunction and the concentration are also specified $\psi = 1$ and $c = 1$ respectively.

4.1 Curved Channel with Stent

For the case when coronary artery has atherosclerosis and drug-eluting stent is placed, the problem is modeled as a parallel and curved plates flow and the stent is modeled by 10 semi-circles uniformly spaced. The geometry used promotes a smooth reduction of length between the bottom and top plates. Were considered 40% of channel obstruction due to atherosclerosis. The Fig. 10 shown velocity field profile along y coordinates in centerline ($x = 5R$).

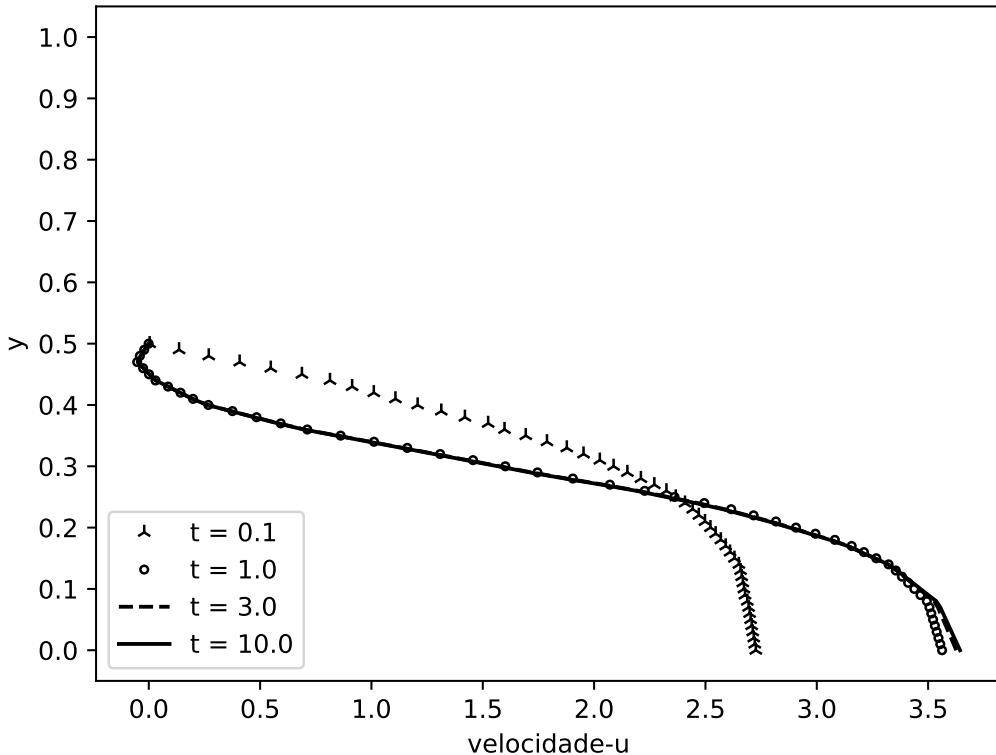


Figure 7: Evolution of velocity profile in time for Curved Channel with Drug-eluting Stent.

In Figs 8 and 9, are shown the velocity and concentration evolution in time and space for half domain according to symmetry y coordinate. The concentration field is represented with non-dimensional values when the red color is $c = 1$ and blue color $c = 0$.

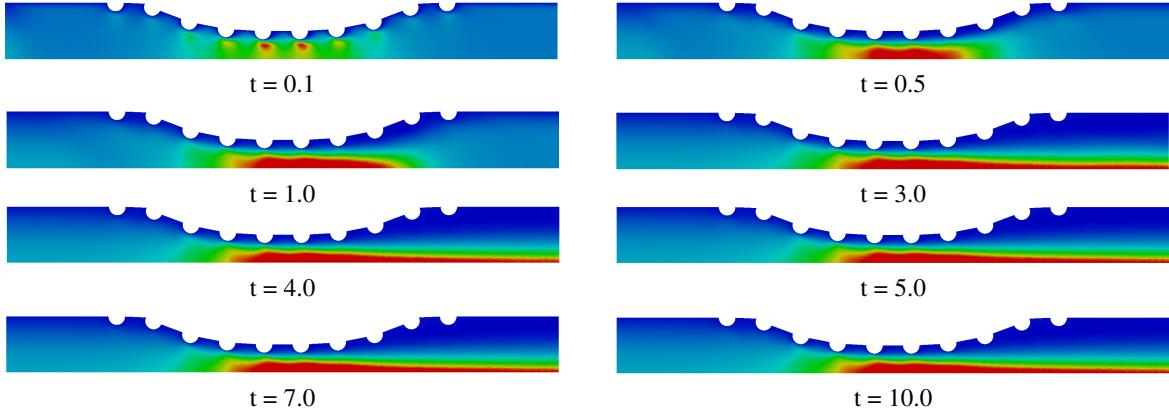


Figure 8: Evolution in time and space of velocity field for Curved Channel with Drug-eluting Stent.

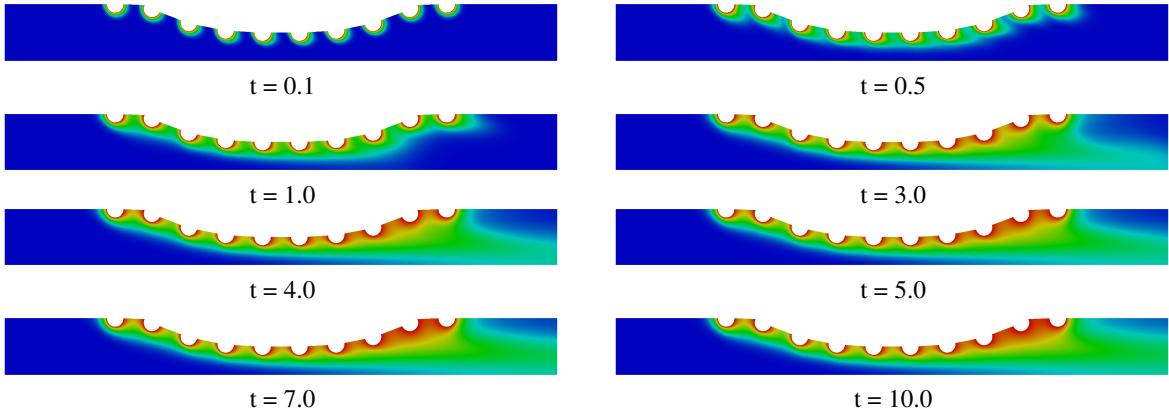


Figure 9: Evolution in time and space of concentration field for Curved Channel with Drug-eluting Stent.

4.2 Real Channel with Stent

In this case, the real coronary artery with atherosclerosis and drug-eluting stent placed is performed. The geometry was taken using image processing from a real coronary artery photography. The stent is modeled by 10 semi-circles uniformly spaced. As in other case, the geometry used promotes a reduction of length between the bottom and top plates when were considered 40% of channel obstruction due to atherosclerosis. The Fig. 10 shown velocity field profile along y coordinates in centerline ($x = 5R$).

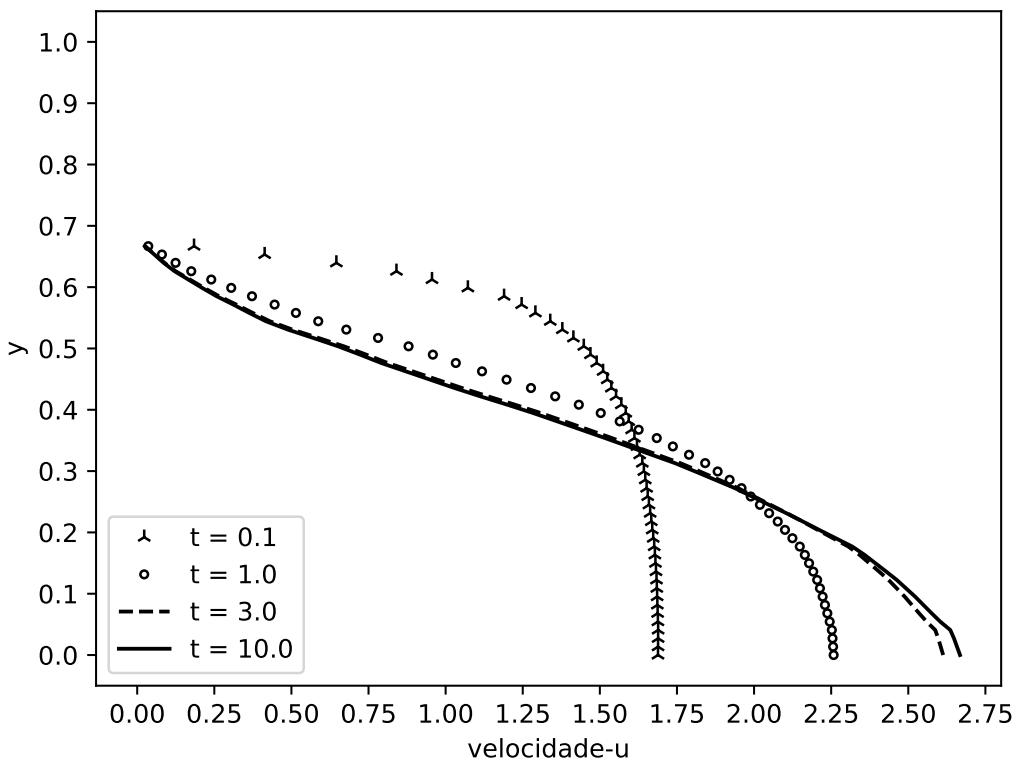


Figure 10: Evolution of velocity profile in time for Curved Channel with Drug-eluting Stent.

In Figs 11 and 12, are shown the velocity and concentration evolution in time and space for half domain according to symmetry y coordinate. The concentration field is represented with non-dimensional values when the red color is $c = 1$ and blue color $c = 0$.

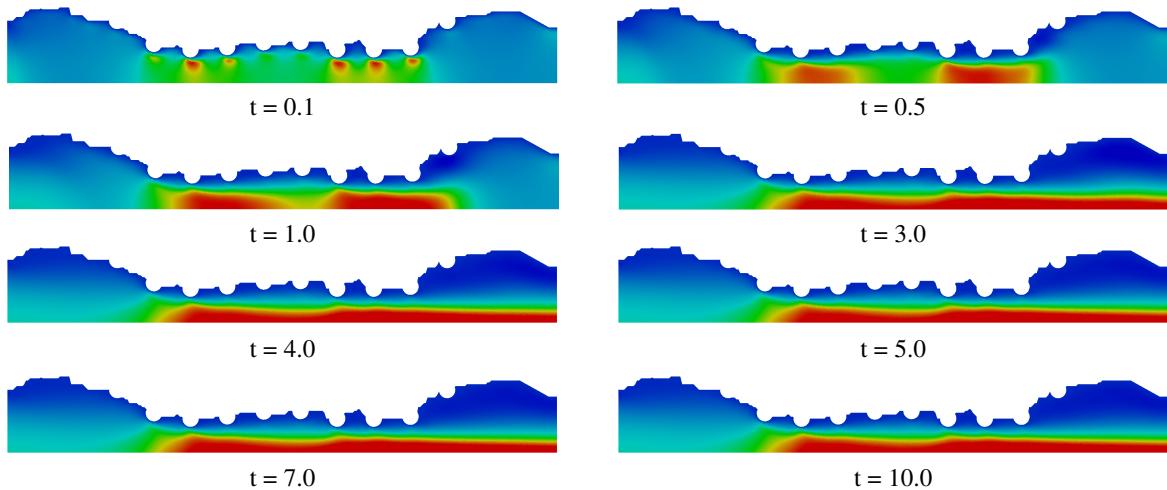


Figure 11: Evolution in time and space of velocity field for Real Channel with Drug-eluting Stent.

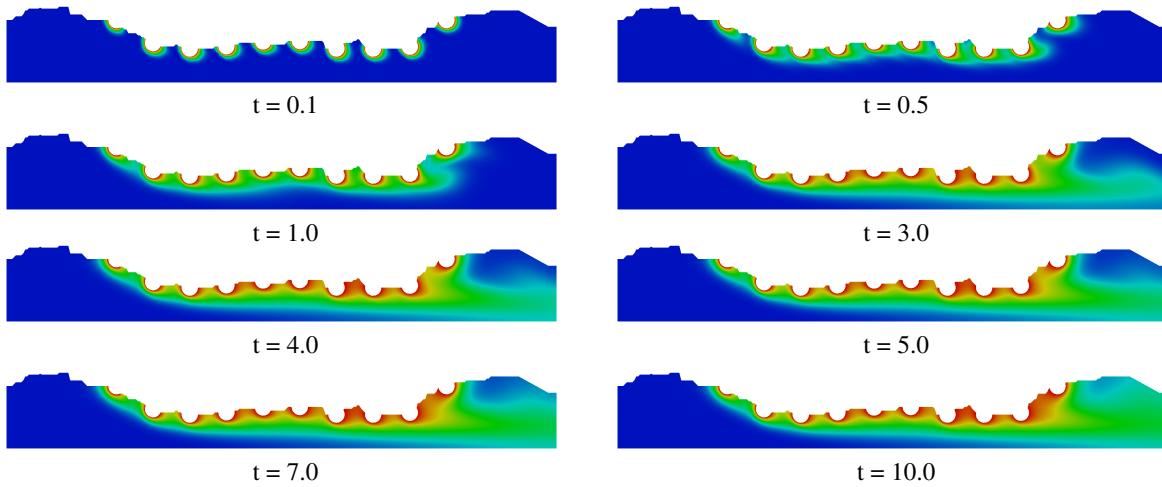


Figure 12: Evolution in time and space of concentration field for Real Channel with Drug-eluting Stent.

5. CONCLUSION

In this work, a numerical code for Navier-Stokes equation according to stream-vorticity formulation with species transport equation coupled was developed using Finite Element Method. The Taylor-Galerkin scheme was applied to decrease the spurious oscillations as seen for moderate to high Reynolds number. The code proved to be effective by results presented in validation cases. The dynamics of blood flow was shown to a coronary artery with atherosclerosis and drug-eluting stent placed. Therefore, the streamfunction and vorticity formulation showed an useful approximation for to calculate the velocity and concentration fields since the variables are scalars allowing then a smooth implementation.

6. ACKNOWLEDGEMENTS

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8. RESPONSIBILITY NOTICE

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A NUMERICAL SIMULATION OF BLOOD FLOW DYNAMICS IN CORONARY ARTERY USING STREAMFUNCTION-VORTICITY FORMULATION

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Abstract: The present work aims at developing a computational framework to simulate coronary artery flows in cartesian coordinates. An accurate method capable of capturing the flow dynamics is strictly required. In this paper a Finite Element Method (FEM) is used to solve the governing equations of the motion of the blood flow found in coronary artery as incompressible fluid using the stream-vorticity formulation with coupled mass transport.

Keywords: Finite Element Method, Taylor-Galerkin Method, Biomedical Engineering, Hemodynamics, Atherosclerosis.

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1. INTRODUCTION

According to the World Health Organization (2017), more people die annually from the cardiovascular diseases (CVDs) than from any other cause in the world. An estimated 17.7 million people died from CVDs in 2015, representing 31% of all global deaths. About 41% of these deaths were due to coronary artery disease (CAD). The leading cause of the CAD is atherosclerosis where the diameter of the vessel is decreased. Two treatments can be performed: coronary artery bypass grafting (CABG) or percutaneous transluminal coronary angioplasty (PTCA). The PTCA is a minimally invasive procedure where a small wire tube, called stents, is placed. This work aims to know how the dynamics of blood flow in coronary artery with atherosclerosis and with stents struts placed.

The dynamics of blood flow in coronary artery and possible influence of stents struts with computational fluid dynamics (CFD) requires a robust numerical method to compute the solution of the differential equations in a relevant model. We consider the model of dissolution and transport of sirolimus on a two-dimensional domain representing the polymer coating layer and the hydrodynamic of the blood flow in the artery in the vicinity of a stent strut as suggested by Bozsak *et al.* (2014) and McGinty and Pontrelli (2016). Also, the effect of the releasing process of the polymers is considered. However, the spatial distribution of the sirolimus is greatly influenced by the flow and the arterial wall properties, being therefore susceptible to patient health conditions. The difference of artery shapes and existence of the struts have been investigated in 4 test cases in the influence on the flow dynamics and the transport of a chemical species as suggested by Wang *et al.* (2017).

We employ the Finite Element method on an unstructured mesh created by open source software called *GMSH* proposed by Geuzaine and Remacle (2009) for the discretization of the incompressible single-phase Navier-Stokes through the stream-vorticity function coupled with the concentration equation. We apply the Taylor-Galerkin method to the decrease the spurious oscillations as seen for moderate to high Reynolds numbers as proposed by Donea (1984) and Zienkiewicz and Taylor (2000) and was used the well-known benchmark problem lid-driven cavity for the validation of the numerical code where the results were compared with Ghia *et al.* (1982) and Marchi *et al.* (2009).

2. MATHEMATICAL MODEL

A 2-dimensional Finite Element Method approach is employed to analyse the dynamics of blood flow in coronary artery and possible influence of stents struts. The first step in its development is the initial modelling of the problem, and in this case it can be described by a formulation using the vorticity and stream function applied in the conservation of momentum equation for incompressible flow and the concentration distribution equation. This approach makes the model useful for the cases of single-phase flows.

$$\frac{\partial w}{\partial t} + \mathbf{v} \cdot \nabla w = \frac{1}{Re} \nabla^2 w \quad (1)$$

$$\nabla^2 \psi = -w \quad (2)$$

$$\mathbf{v} = \mathbf{D}\psi \quad (3)$$

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \frac{1}{ReSc} \nabla^2 c \quad (4)$$

Where, ω is the vorticity field, ψ is the stream function field, c is the concentration field, $\mathbf{v} = (u, v)$ is the velocity field, $\mathbf{D} = [\partial/\partial y, -\partial/\partial x]$ is a mathematical operator, $Re = \rho u D / \mu$ is the Reynolds number, $Sc = \nu/D$ is the Schmidt number, x and y are the independent spatial variables and t is the time variable.

2.1 Initial and Boundary Conditions

As commented by Anjos (2012), the initial conditions and the boundary conditions are of utmost importance to realistically characterizing any problem modeled by differential equations. Thus, the boundary conditions used in this paper are briefly explained below:

- *inflow condition*: the normal velocity component is set to null value $v = 0$. The derivates of the streamfunction and the concentration are set null values $\partial\psi/\partial n = 0$ and $\partial c/\partial n = 0$ respectively. For the tangent velocity component is set a half parabolic profile comes from the analytical solution of a Straight Channel in the cartesian coordinates: $u = u_{max}(1 - (y/R)^2)$, where $u_{max} = 2$.
- *No-slip condition*: all the velocity components are specified with null value $u = 0$ and $v = 0$. The streamfunction is also specified $\psi = 1.3$. The derivative concentration is set null value $\partial c/\partial n = 0$.
- *outflow condition*: no value is specified. The derivatives of the tangent velocity component, of the normal velocity component, of streamfunction and of concentration are set to null values, that is, $\partial u/\partial n = 0$, $\partial v/\partial n = 0$, $\partial\psi/\partial n = 0$ and $\partial c/\partial n = 0$ respectively.
- *Free-slip condition*: used when a symmetry condition is desired. The normal velocity component is set to null value $v = 0$ as well as the streamfunction $\psi = 0$. The derivative of the tangent velocity component and the derivative of the concentration are also set to null value $\partial u/\partial n = 0$ and $\partial c/\partial n = 0$ respectively.
- *Strut condition*: used on the stent. The normal velocity component and the tangent velocity component are specified with null value $u = 0$ and $v = 0$. The streamfunction and the concentration are also specified $\psi = 1.3$ and $c = 1$ respectively.

The boundary condition of the vorticity field is calculated in the solution algorithm scheme as we will see later.

2.2 Finite Element Method

This is paper, was used the Galerkin formulation to discretize the government equations. The spatial domain was discretized using linear triangular elements by open source software called GMSH proposed by Geuzaine and Remacle (2009). For the discretization of the temporal domain was used a finite differences method with a forward difference approximation and the Taylor-Galerkin Method with omitted terms of higher order than two was used to the decrease the spurious oscillations for moderate to high Reynolds numbers as proposed by Donea (1984) and Zienkiewicz and Taylor (2000). Therefore, the governing equations in matrix form used in this paper were:

$$\left[\frac{M}{\Delta t} + \frac{1}{Re} [K_{xx} + K_{yy}] \right] w^{n+1} = \frac{M}{\Delta t} w^n - u \cdot G_x w^n - v \cdot G_y w^n - u \frac{\Delta t}{2} [u K_{xx} + v K_{xy}] w^n - v \frac{\Delta t}{2} [u K_{yx} + v K_{yy}] w^n \quad (5)$$

$$[K_{xx} + K_{yy}] \psi = M w \quad (6)$$

$$M u = G_y \psi \quad (7)$$

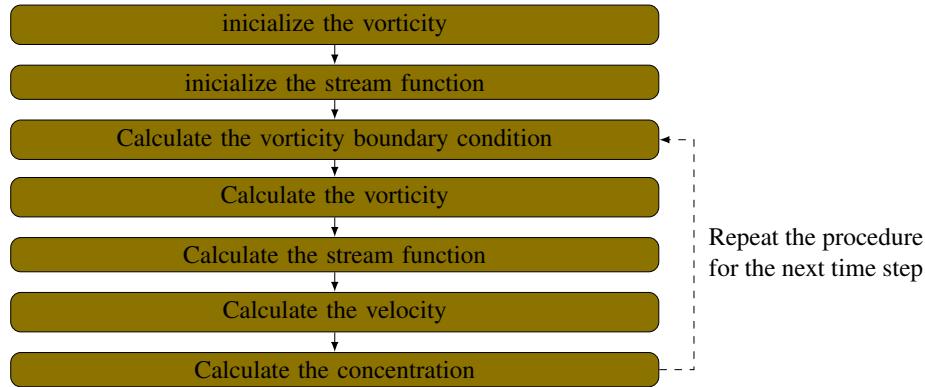
$$Mv = -G_x \psi \quad (8)$$

$$\left[\frac{M}{\Delta t} + \frac{1}{ReSc} [K_{xx} + K_{yy}] \right] c^{n+1} = \frac{M}{\Delta t} c^n - u \cdot G_x c^n - v \cdot G_y c^n - u \frac{\Delta t}{2} [u K_{xx} + v K_{xy}] c^n - v \frac{\Delta t}{2} [u K_{yx} + v K_{yy}] c^n \quad (9)$$

Where, M is mass matrix, G_x and G_y are gradient matrix, K_{xx} , K_{xy} , K_{yx} and K_{yy} are stiffness matrix. The last term of the Eqs. 5 and 9 is known as numerical diffusion and it decrease the spurious oscillations as seen for moderate to high Reynolds numbers. For scalars, *Taylor Galerkin Method* and *Characteristic Galerkin* produce the same result as showed by Lohner *et al.* (1984). The superscripts $n+1$ and n are the scalar that will be calculated and that was calculated in the previous time step, respectively.

2.3 Numerical Solution

The linear system of equations that come from implementing the FEM is solved through iterative method *Conjugate Gradient Solver* available in the public library for scientific tools *SciPy* maintained by Jones *et al.* (2001) in the Python language. The solution algorithm used is shown below:



that is:

1. Initialize the vorticity with the equation:

$$Mw = G_x v - G_y u$$

2. Initialize the stream function with the equation:

$$[K_{xx} + K_{yy}] \psi = Mw$$

It is necessary to apply the boundary condition in the equation.

3. Calculate the vorticity boundary condition with the equation:

$$Mw = G_x v - G_y u$$

4. Calculate the vorticity with the equation:

$$\left[\frac{M}{\Delta t} + \frac{1}{Re} [K_{xx} + K_{yy}] \right] w^{n+1} = \frac{M}{\Delta t} w^n - u \cdot G_x w^n - v \cdot G_y w^n - u \frac{\Delta t}{2} [u K_{xx} + v K_{xy}] w^n - v \frac{\Delta t}{2} [u K_{yx} + v K_{yy}] w^n$$

Where w^n is the vorticity calculated in the previous time step and w^{n+1} is the vorticity that will be calculated in the time step. It is necessary to apply the boundary condition calculated in the third step before finding vorticity field.

5. Calculate the stream function with equation:

$$[K_{xx} + K_{yy}] \psi = Mw$$

It is necessary to apply the boundary condition in the equation before finding streamfunction field.

6. Calculate the velocity with the equation:

$$Mu = G_y \psi$$

$$Mv = -G_x \psi$$

It is necessary to apply the boundary condition in the equation before u and v . Note that one can solve the linear system using the conjugate gradient method, since M is positive and definite matrix or M can be approximated by its lumped version and therefore easily inverted.

7. Calculate the concentration with equation:

$$\left[\frac{M}{\Delta t} + \frac{1}{ReSc} [K_{xx} + K_{yy}] \right] c^{n+1} = \frac{M}{\Delta t} c^n - u \cdot G_x c^n - v \cdot G_y c^n \\ - u \frac{\Delta t}{2} [u K_{xx} + v K_{xy}] c^n - v \frac{\Delta t}{2} [u K_{yx} + v K_{yy}] c^n$$

Where c^n is the vorticity calculated in the previous time step and c^{n+1} is the vorticity that will be calculated in the time step. It is necessary to apply the boundary condition in the equation before finding concentration field.

8. Return the third step and repeat the procedure for next time step.

The first and second steps are out of time loop, while the third to the seventh step are inside of time loop. The application of the boundary condition in the equation can be before loop, except for the vorticity equation (*fourth step*) that the boundary condition must be applied at each time step.

3. VALIDATION

The validation of the numerical simulation was done by well-known benchmark problem: flow in a lid-driven cavity. The dimensions domain in x-direction and y-direction are [0,1]. We used a mesh with 1563 nodes and 2988 elements and the following Reynolds numbers (Re): 10, 100, 400 and 1000. The results were compared with Ghia *et al.* (1982) and Marchi *et al.* (2009).

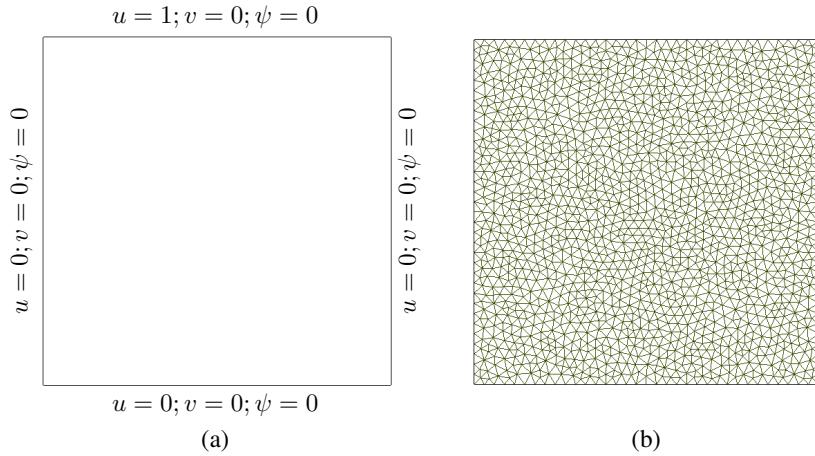


Figure 1: Lid-driven cavity: (a) geometry (b) mesh.

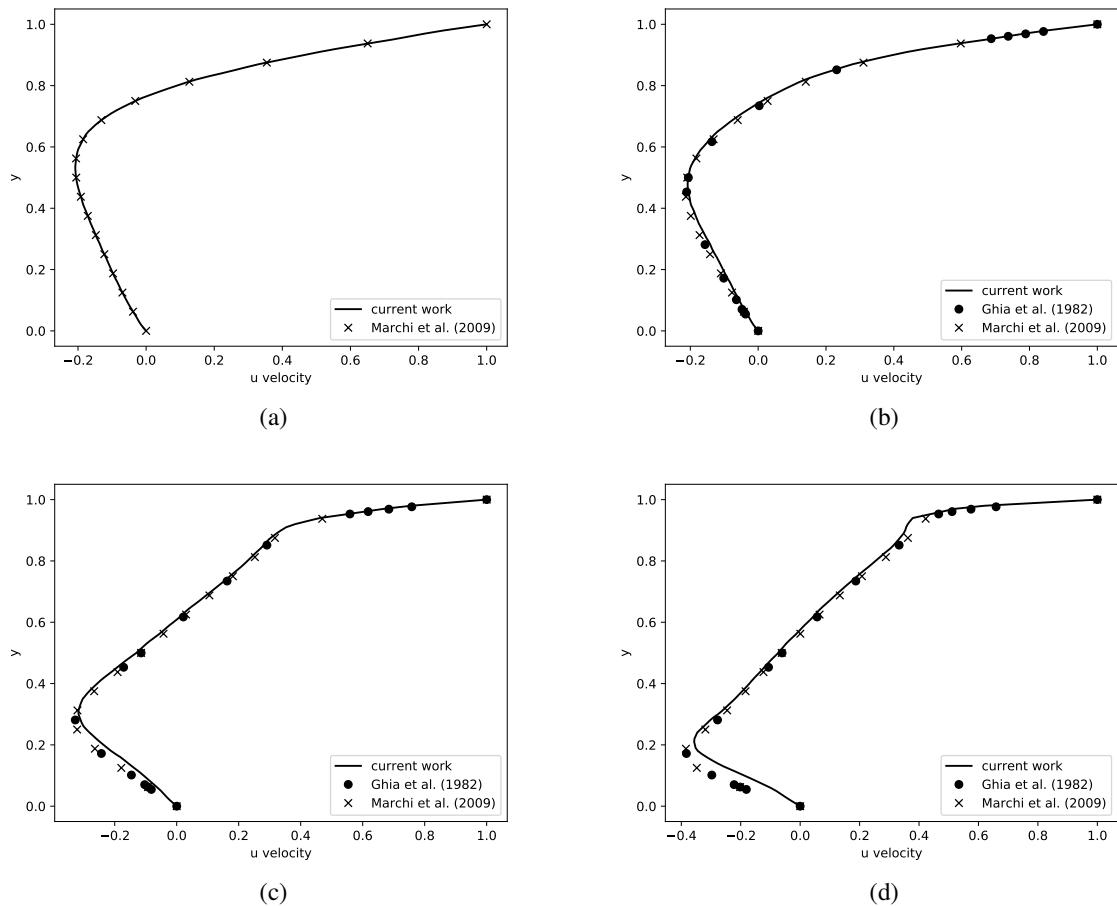


Figure 2: Centerline velocity profile ($x = 0.5$) in a lid-driven cavity for different Reynolds numbers: (a) 10 (b) 100 (d) 400 (f) 1000.

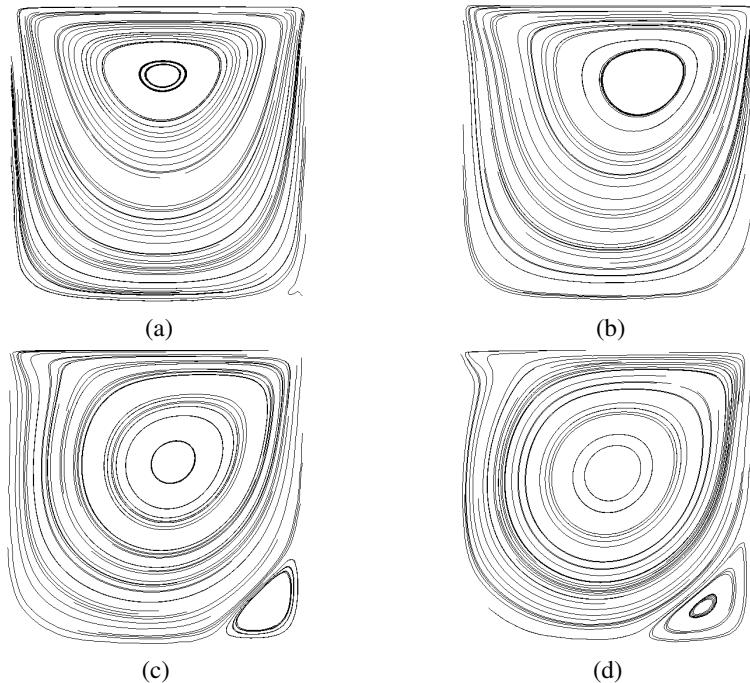


Figure 3: Streamfunction countours in a lid-driven cavity for different Reynolds numbers: (a) 10 (b) 100 (c) 400 (d) 1000.

4. RESULTS AND DISCUSSION

Some results of simulations are shown to demonstrate its capability of using unstructured triangular meshes on various geometries and combination of geometries. Numerical results are given for several cases of blood flows in artery. The post-processing was performed by open source software *PARAVIEW* proposed by Henderson (2007). The lumen diameter of a typical artery is about $D = 0.003\text{m}$, viscosity in the lumen are set to $\mu = 0.0035\text{Pa.s.}$ and density $\rho = 1060\text{kg/m}^3$ as suggested by Bozsak *et al.* (2014). According to Kessler *et al.* (1998), the velocity of the flow at coronary artery is $v = 12\text{cm/s.}$ Therefore, the Reynolds number is $Re = 109.$ Four different geometries were used in the simulations as proposed by Wang *et al.* (2017) and is shown in the Figure 4. Only half domain are shown since the results are symmetric in y-direction.

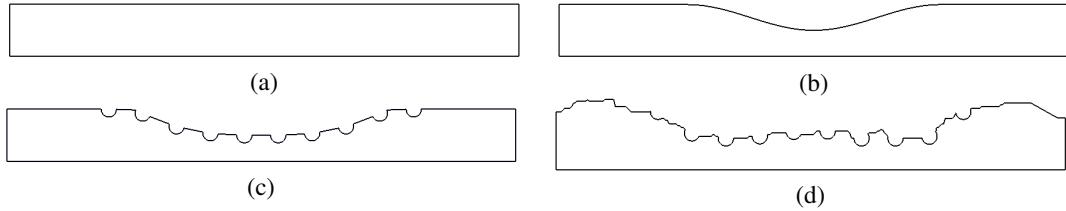


Figure 4: Non-dimensional geometry for blood flow dynamics in coronary arteries. The channel length $L = 10R$ is based on the channel width $R = 1.$ (a) Straight Channel (b) Curved Channel (c) Curved Channel with Stent and (d) Real Channel with Stent.

4.1 Straight Channel

For the case where we don't have atherosclerosis, the coronary artery is a straight channel. In the literature, this case is known as Hagen-Poiseuille flow and there is an analytical solution for the velocity profile. The analytical solution is given by:

$$u = u_{max} \left(1 - \frac{y^2}{R^2} \right) \quad (10)$$

where u_{max} is the velocity in the symmetry axis and has the value $u_{max} = 2,$ R is non-dimensional radius and has the value $R = 1$ and y the width of half vessel and ranges from $y = [0, 1].$

The Figure 5 shows the transient velocity profile along the y-direction at the middle of the channel ($x = 5.0R$). As expected, the velocity profile evolution in time converges to the analytical solution with a small error.

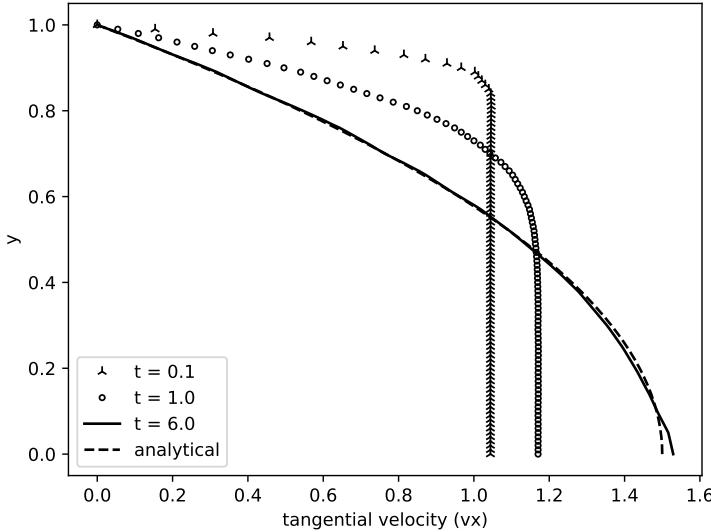


Figure 5: Velocity field profile evolution in time for Straight Channel.

The Figure ?? shows the velocity field evolution in space and time for half domain since the results are symmetric in y-direction. The velocity field is represented with non-dimensional values where the red color is $vx = 2$ and the blue color is $vx = 0.$

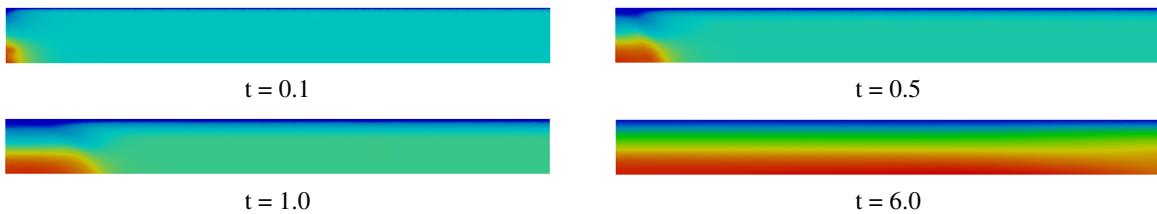


Figure 6: Time evolution of the velocity field for the straight geometry channel. The velocity profile at the middle of the channel is showed in Fig. 5.

4.2 Curved Channel

For the case where we have atherosclerosis, the coronary artery is a curved channel. This geometry promotes a smooth reduction of the channel diameter followed by a smooth expansion as commonly found in Venturi channel. Was considered 40% of obstruction, that is, the vessel has 60% of diameter for blood flow. The Figure 7 shows the transient velocity profile along the y-direction at the middle of the channel ($x = 5.0R$).

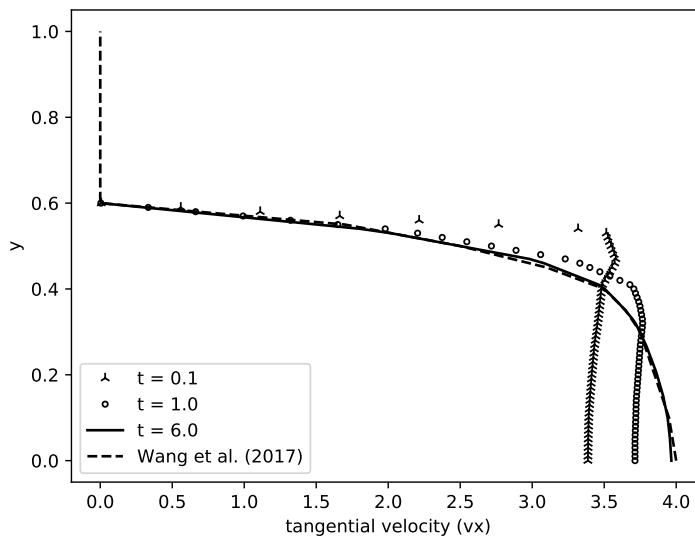


Figure 7: Velocity field profile evolution in time for Curved Channel.

The Figure 8 shows the velocity field evolution in space and time for half domain since the results are symmetric in y-direction. The velocity field is represented with non-dimensional values where the red color is $vx = 4$ and the blue color is $vx = 0$.



Figure 8: Time evolution of the velocity field for the curved geometry channel. The velocity profile at the middle of the channel is showed in Fig. 7.

4.3 Curved Channel with Stent

In this case, the stent strut was placed at the top of the curved channel and it was modeled by 10 semi-circles uniformly spaced. As in other cases was considered 40% of obstruction, that is, the vessel has 60% of diameter for blood flow. The Figure 9 shows the transient velocity profile along the y-direction at the middle of the channel ($x = 5.0R$).

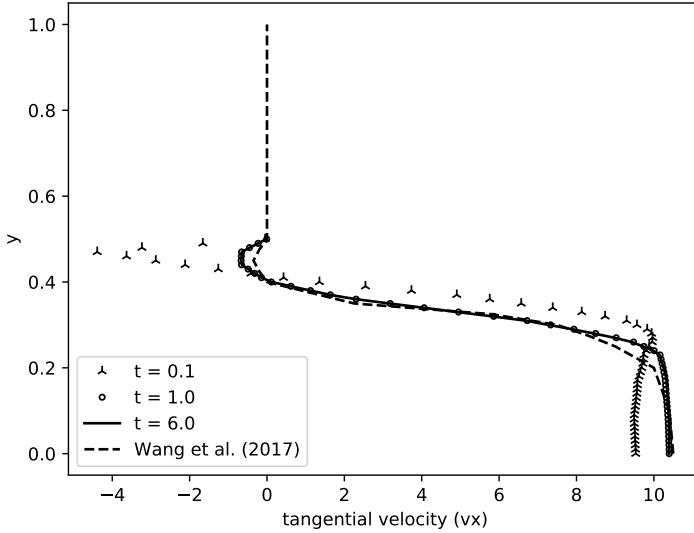


Figure 9: Velocity field profile evolution in time for Curved Channel with Stent.

The Figure 10 shows the velocity field evolution in space and time on the left hand side and the concentration field evolution on the right hand side for half domain since the results are symmetric in y -direction. The velocity field is represented with non-dimensional values where the red color is $vx = 10$ and the blue color is $vx = 0$. The concentration field also is represented with non-dimensional values where the red color is $c = 1$ and the blue color is $c = 0$.

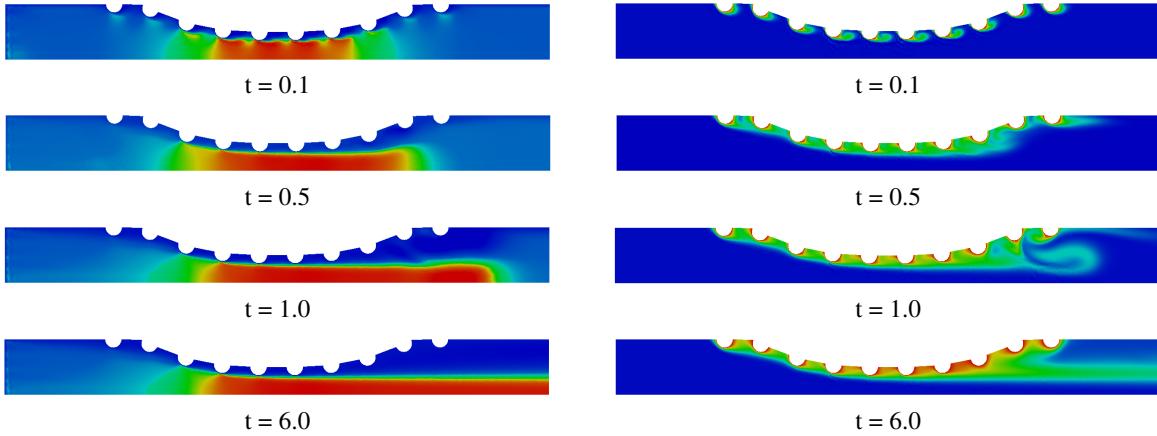


Figure 10: Time evolution of the velocity (left) and concentration (right) fields for the curved geometry channel with stent strut. The velocity profile at the middle of the channel is showed in Fig. 9.

4.4 Real Channel with Stent

In this case, a numerical simulation was performed for a real artery channel whose geometry was taken using image processing from a real coronary artery photography as proposed by Wang *et al.* (2017). It is important to know that each coronary artery geometry is particular to each patient and compatible to its health conditions. The stent strut was placed at the top of the curved channel and it was modeled by 10 semi-circles uniformly spaced. As in other cases was considered 40% of obstruction, that is, the vessel has 60% of diameter for blood flow. The Figure 11 shows the transient velocity profile along the y -direction at the middle of the channel ($x = 5.0R$).

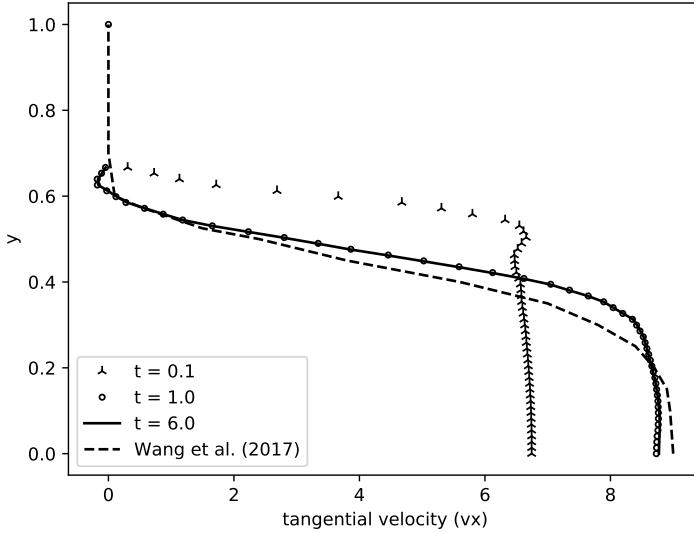


Figure 11: Velocity field profile evolution in time for Real Channel with Stent.

The Figure 12 shows the velocity field evolution in space and time on the left hand side and the concentration field evolution on the right hand side for half domain since the results are symmetric in y -direction. The velocity field is represented with non-dimensional values where the red color is $vx = 9$ and the blue color is $vx = 0$. The concentration field also is represented with non-dimensional values where the red color is $c = 1$ and the blue color is $c = 0$.

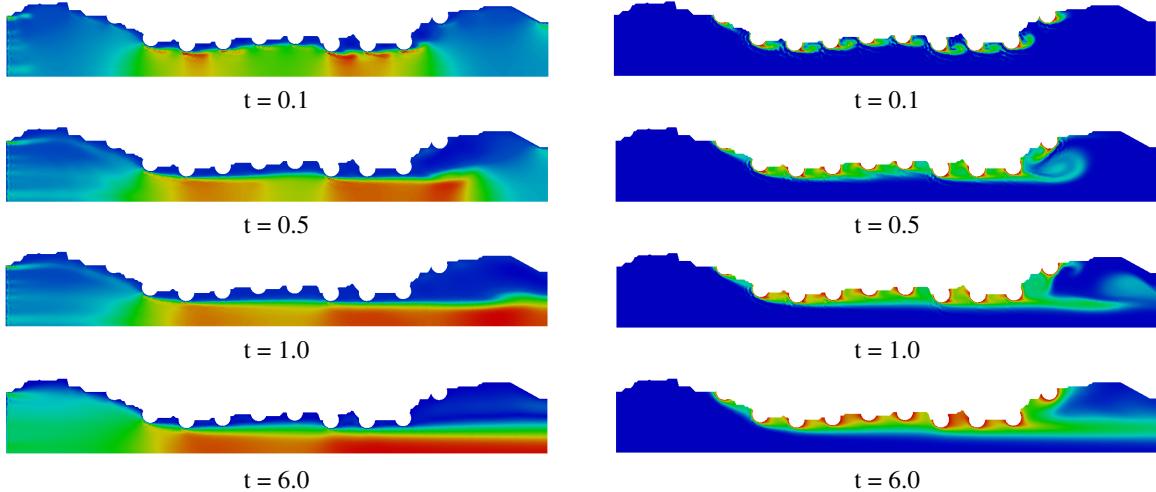


Figure 12: Time evolution of the velocity (left) and concentration (right) fields for the curved geometry channel with stent strut. The velocity profile at the middle of the channel is showed in Fig. 11.

5. CONCLUSION

The results obtained in this paper for the velocity and concentration fields of complex geometries of a modeled coronary artery channel were similar to those presented by Wang *et al.* (2017). However, the numerical simulation was performed using the streamfunction and vorticity formulation by finite element method approach. The Taylor-Galerkin Method was applied to the decrease the spurious oscillations as seen for moderate to high Reynolds numbers. The validation of the numerical solution was done by well-known benchmark lid-driven cavity problem and the results were compared with others authors as well as the Hagen-Poiseuille flow for the case straight channel that was compared with analytical solution. The streamfunction and vorticity formulation showed an useful approximation for to calculate the velocity and concentration fields since the variables are scalars allowing then a smooth implementation.

6. ACKNOWLEDGEMENTS

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8. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.

BLOOD FLOW SIMULATION USING STREAM FUNCTION-VORTICITY FEM FORMULATION

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1. ABSTRACT

The present work aims at developing a computational framework to simulate coronary artery flows in cartesian coordinates. An accurate method capable of capturing the flow dynamics is strictly required. In this paper a Finite Element Method (FEM) is used to solve the governing equations of the motion of the blood flow found in coronary artery as incompressible fluid using the stream-vorticity formulation with coupled species transport equation.

Keywords: Finite Element Method, Taylor-Galerkin Method, Coronary Artery, Blood.

2. INTRODUCTION

According to the *Health World Organization*, more people die annually from the cardiovascular diseases (CVDs) than from any other cause in the world. The leading cause of these deaths is coronary artery with atherosclerosis and the main purpose of stent implementation is to attack this problem. This work aims to know how the dynamics of blood flow in coronary artery with atherosclerosis and with stents struts placed.

We consider the hydrodynamic of the blood flow in the artery in the vicinity of a stent strut for a two-dimensional domain. The difference of artery shapes and existence of the struts have been investigated in 4 test cases in the influence on the flow dynamics and the transport of chemical species as suggested by Wang et al. (2017).

We employ the Finite Element method on an unstructured mesh created by open source software called *GMSH* for the discretization of the incompressible single-phase Navier-Stokes through the stream-vorticity function coupled with species transport equation. We apply the Taylor-Galerkin method to the decrease the spurious oscillations as seen for moderate to high Reynolds numbers as proposed by Donea (1984).

3. MATHEMATICAL MODEL

A two-dimensional Finite Element Method approach is employed to analyse the dynamics of blood flow in coronary artery and possible influence of stents struts. The modelling of the problem can be described by a formulation using the vorticity and stream function applied in the conservation of momentum equation for incompressible flow and the species transport equation.

$$\frac{\partial \omega}{\partial t} + \mathbf{v} \cdot \nabla \omega = \frac{1}{Re} \nabla^2 \omega \quad (1)$$

$$\nabla^2 \psi = -\omega \quad (2)$$

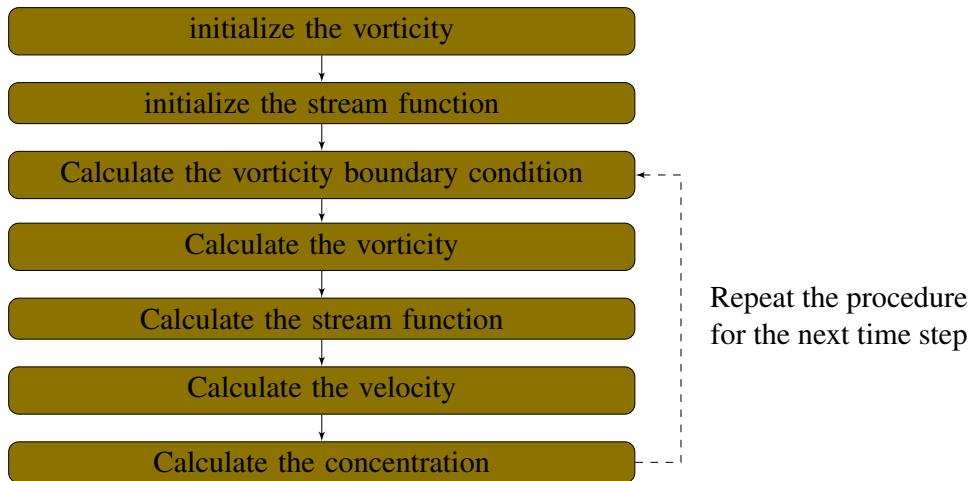
$$\mathbf{v} = \mathbf{D}\psi \quad (3)$$

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \frac{1}{ReSc} \nabla^2 c \quad (4)$$

Where ω is the vorticity field, ψ is the stream function field, c is the concentration scalar field of the chemical species, $\mathbf{v} = (v_x, v_y)$ is the velocity field, $\mathbf{D} = [\partial/\partial y, -\partial/\partial x]$ is a mathematical operator, $Re = \rho u D / \mu$ is the Reynolds number, $Sc = \nu/D$ is the Schmidt number, x and y are the independent spatial variables and t is the time variable.

The temporal domain was discretized using the Taylor series with the terms higher second order omitted. The second order terms were used to decrease the spurious oscillations for moderate to high Reynolds numbers as proposed by Donea (1984). The spatial domain was discretized by Galerkin Formulation using linear triangular.

The linear system of equations that come from implementing the FEM is solved through an iterative method *Conjugate Gradient Solver* available in the public library for scientific tools *SciPy* in the *Python language*. The solution algorithm used is shown below:



4. RESULTS

Numerical results are shown for several cases of blood flows in artery. The post-processing was performed by open source software *PARAVIEW*. The lumen radius of a typical artery is about $R = 0.0015\text{m}$, viscosity in the lumen are set to $\mu = 0.0035\text{Pa.s.}$ and density $\rho = 1060\text{kg/m}^3$ as suggested by Bozsak et al. (2014). According to Kessler et al. (1998), the velocity of the flow at coronary artery is $v = 12\text{cm/s.}$ Therefore, the Reynolds number is $Re = 54.5.$ Four non-dimensional geometries were used with channel length $L = 10R$ and channel width $R = 1$ as proposed by Wang et al. (2017), however were modified to cartesian coordinates and

are shown in the Figure 1. Only half domain are shown since the results are symmetric in y -direction.

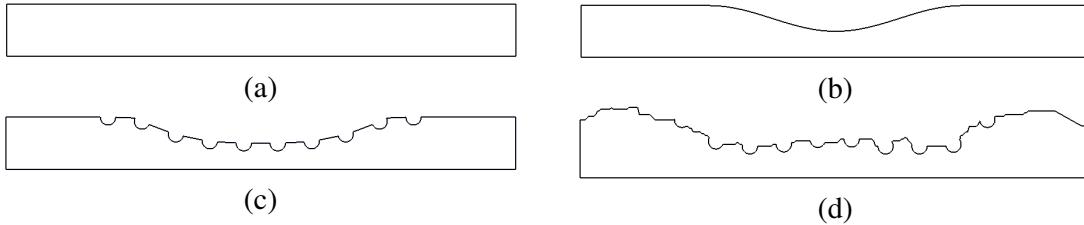


Figura 1 – Non-dimensional geometry for blood flow dynamics in coronary arteries. (a) Straight Channel (b) Curved Channel (c) Curved Channel with Stent and (d) Real Channel with Stent.

In fig 2 and 3, are shown the velocity profiles evolution in time and the velocity and concentration fields for the steady state respectively. There is a significant difference between the results shown and those shown in axisymmetric coordinates by Wang et al. (2017).

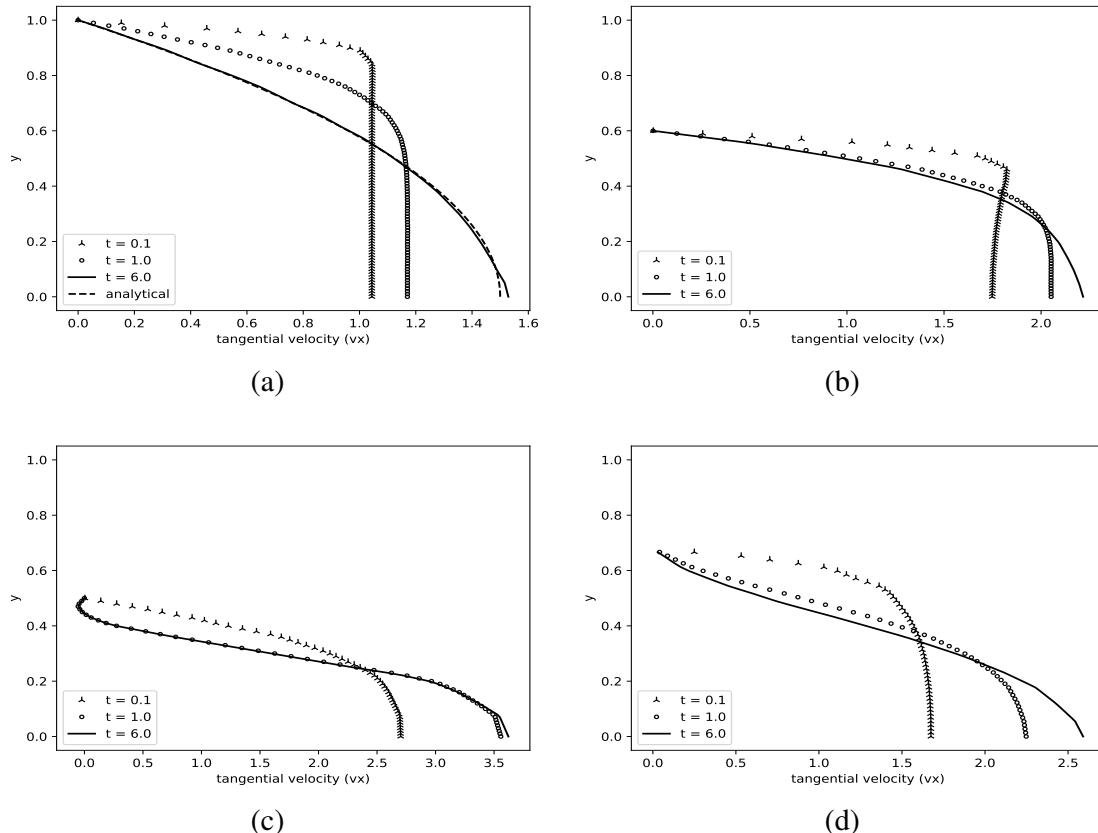


Figura 2 – Velocity field profile evolution in time for various geometries (a) Straight Channel (b) Curved Channel (c) Curved Channel with Stent and (d) Real Channel with Stent.

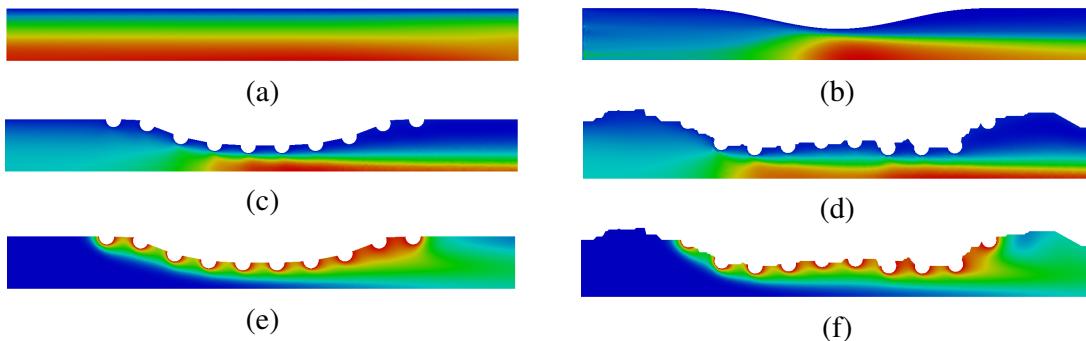


Figura 3 – Velocity field steady state: (a) Straight Channel (b) Curved Channel (c) Curved Channel with Stent and (d) Real Channel with Stent. Concentration field steady state: (e) Curved Channel with Stent and (f) Real Channel with Stent.

5. CONCLUSION

In this paper, the results were shown for two-dimensional domain in complex geometries of modeled coronary artery channel. The numerical simulation was performed using the streamfunction and vorticity formulation with coupled species transport equation by finite element method approach. The streamfunction and vorticity formulation showed a smooth implementation for to calculate the variables since they are scalars. However, there is a significant difference between the results shown in cartesian coordinates and those shown by Wang et al. (2017) in axisymmetric coordinates.

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