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BLOOD FLOW NUMERICAL SIMULATION USING FE METHOD FOR 2D-AXISYMMETRIC NAVIER-STOKES EQUATION

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Abstract. *According to the World Health Organization, more people die annually from the cardiovascular disease (CVD) that from any other cause in the world. About 44% of these deaths were due to coronary heart disease (CHD) in the United States. This work aims to develop a FE code for 2D Axisymmetric Navier-Stokes with species transport equation using semi-Lagrangian scheme and to know how occurs the dynamics of blood flow in coronary artery with atherosclerosis and with stents struts placed. The blood was modeled as single-phase, incompressible and newtonian fluid, the diffusion coefficient was considered as constant. Due to coupling between velocity field and pressure field, the different triangular elements was used, where the linear element was used for pressure field and the MINI element was used for velocity field. The equations were discretized in space by Galerkin formulation and in time, the semi-Lagrangian scheme was used to discretized the material derivative using first order backward difference scheme. The dynamics of blood flow and species transport in coronary artery was investigated in a complex geometry, that it was called the Curved Channel with Stent, where the atherosclerosis was modeled using a sinusoidal equation to model 40% of channel obstruction. The Reynolds number was calculated using the blood parameters and the Schmidt number was simulated for several cases.*

Keywords: *Navier-Stokes, Axisymmetric, Finite Element Method, Semi-Lagrangian, Drug-Eluting Stent.*

1. INTRODUCTION

According to the World Health Organization (2017), more people die annually from the cardiovascular disease (CVD) that from any other cause in the world. An estimated 17.9 million people died from CVD in 2016, representing 31% of all global deaths. About 44% of these deaths were due to coronary heart disease (CHD) in the United States (Benjamin *et al.*, 2018). According to the Barquera *et al.* (2015), the leading cause of the CHD is atherosclerosis where the diameter of the vessel is decreased and the best treatments is the lifestyle change. For a corrective approach, however, 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 an FE code for 2D Axisymmetric Navier-Stokes Equation with species transport equation using semi-Lagrangian scheme and to know how occurs 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 in an Eulerian context. The blood was modeled as single-phase, incompressible and newtonian fluid, the diffusion coefficient was considered as constant. The Navier-Stokes equation is shown with species transport equation in a Finite Element Method approach.

The domain was discretized on an unstructured triangular mesh using the *GMSH* open source. Due to coupling between velocity field and pressure field, the different triangular elements was used, where the linear element was used for pressure field and the *MINI* element was used for velocity field. Therefore, the Babuska-Brezzi restriction was respected (Babuska (1971) and Brezzi (1974)). In addition, the *Mini* element was also used in the concentration field. The equations were discretized in space by Galerkin formulation and in time, the semi-Lagrangian scheme was used to discretized the material derivative using first order backward difference scheme.

The linear system of equations that comes from implementing the FEM is solved throught iterative method *Conjugate Gradient Solver* available in the public library for scientific tools *SciPy*. The dynamics of blood flow and species transport in coronary artery was investigated in a complex geometry, called the *Curved Channel with Stent*, where the atherosclerosis was modeled using a sinusoidal equation to model 40% of channel obstruction. The Reynolds number was calculated using the blood parameters and the Schmidt number was simulated for several cases.

2. MATHEMATICAL MODEL

A 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 in an Eulerian context. The blood was modeled as single-phase, incompressible and newtonian fluid, the diffusion coefficiente was considered as constant. The Navier-Stokes equation is shown with species transport equation in an Eulerian 2D-Axisymmetric approach:

$$\frac{\partial V_r}{\partial r} + \frac{\partial V_z}{\partial z} + \frac{V_z}{r} = 0$$

$$\frac{\partial V_r}{\partial t} + u\frac{\partial V_r}{\partial r} + v\frac{\partial V_r}{\partial z} = -\frac{\partial p}{\partial r} + \frac{1}{Re}\left(\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial V_r}{\partial r} + \frac{\partial^2 V_r}{\partial z^2} - \frac{2V_r}{r}\right)$$

$$\frac{\partial V_z}{\partial t} + u\frac{\partial V_z}{\partial r} + v\frac{\partial V_z}{\partial z} = -\frac{\partial p}{\partial z} + \frac{1}{Re}\left(\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial V_z}{\partial r} + \frac{\partial^2 V_z}{\partial z^2}\right)$$

$$\frac{\partial e}{\partial t} + u\frac{\partial e}{\partial r} + v\frac{\partial e}{\partial z} = \frac{1}{ReSc}\left(\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial e}{\partial r} + \frac{\partial^2 e}{\partial z^2}\right)$$

(1)

where, V_r is the r-coordinate velocity component (radial component), V_z is the z-coordinate velocity component (tangential component), p is the pressure field, e is the concentration field, $Re = \rho u R/\mu$ is the Reynolds number, where ρ is the blood density (kg/m^3), u is the blood velocity in the coronary artery (m/s), R is the lumen radius of the coronary artery (m) and μ is the blood viscosity (N.s/m^2), $Sc = \mu/\rho D$ is the Schmidt number, where D is the mass diffusion rate of the drug (m^2/s) and r and z are the spatial variables.

The boundaries conditions used were:

- *inflow condition*: this condition was specified in the left line of the geometries in this work, where an mass inflow is desired. For such a condition, $V_r = v_o$ and $V_z = u_o$, where $u_o = 2[1 - (r/R)^2]$ and $v_o = 0$

- *wall condition*: this condition is specified at wall boundary, that is, the top line of the geometries in this work, where the no-slip condition is set. All the velocity components are specified with null values.

- *outflow condition*: this condition represents a state where is close to a fully developed profile, that is, the right line of the geometries in this work. For this condition, the pressure field is set as $p = 0$.

- *free-slip condition (symmetry)*: this condition is specified at the symmetric axis, that is, the bottom line of the geometries in this work. The radial velocity component is null and the derivative of the tangential component is also null value.

- *strut condition (semi-circles)*: this condition is used on the semi-circles of drug-eluting stent. The radial and tangential velocity components are specified with null value. The concentration field is specified as $e = e_o$, where $e_o = 1$.

2.1 Galerkin Method

The domain was discretized on an unstructured triangular mesh using the *GMSH* open source. Due to coupling between velocity field and pressure field, the different triangular elements was used, where the linear element was used for pressure field and the *MINI* element was used for velocity field. Therefore, the Babuska-Brezzi restriction was respected (Babuska (1971) and Brezzi (1974)). In addition, the *Mini* element was also used in the concentration field. The convective term of Eq. 1 will be replaced by material derivative for further time discretization using semi-Lagrangian Method. For spatial discretization of governing equations, the Galerkin method was used, resulting in the following matrix system:

$$D_r V_r + \left(D_z + M_{1/r}\right) V_z = 0 \tag{2}$$

$$M \frac{DV_r}{Dt} + \frac{1}{Re} \left(K + 2M_{1/r}\right) V_r - G_r p = 0 \tag{3}$$

$$M \frac{DV_z}{Dt} + \frac{1}{Re} K V_z - G_z p = 0 \tag{4}$$

$$M \frac{De}{Dt} + \frac{1}{ReSc} K e = 0 \tag{5}$$

where, M is mass matrix, $M_{1/r}$ is mass matrix with 1/r in elementary matrix, K are stiffness matrix. In this moment, the velocity (u, v), the pressure p and the drug concentration field e fields are discretized in the spatial domain but continuos in the temporal domain. Then, for time discretization, the semi-Lagrangian Method was used.

2.2 Semi-Lagrangian Scheme

The Semi-Lagrangian Scheme in centred difference was proposed by Sawyer (1963) for atmospheric flow numerical simulation using vorticity-advection equation, allowing to use large time steps without numerical instability. However, because of a limited computer capability, the use of such methodology to model several fluid flow problems, with high order differences and fine mesh, came latter in the 1980's throught the work of Robert (1981) and Pironneau (1982), where the semi-lagrangian scheme would be able to run models faster than the Eulerian scheme, besides be unconditionally stable and only symmetric linear systems to solve. Basically, the semi-lagrangian scheme takes into account the fact that the Eulerian derivative is replaced by the material derivative, then it is discretized and computed along the trajectory characteristic:

$$\frac{D\mathbf{v}}{Dt} \approx \frac{\mathbf{v}_i^{n+1} - \mathbf{v}_d^n}{\Delta t} \tag{6}$$

where, $D\mathbf{v}/Dt$ is material derivative of $\mathbf{v}$ and the right-hand side equation is material derivative discretized using first order backward difference scheme. The variable t is time, $\mathbf{v}_i^{n+1}$ is the velocity field calculated in current time step at the current node position and $\mathbf{v}_d^n$ is the velocity field calculated in previous time step at the departure node position.

The departure node is found by solving equation $\mathbf{x}_d^n = \mathbf{x}_i^{n+1} - \mathbf{v}\Delta t$, using the initial condition $\mathbf{x}_i^{n+1} = \mathbf{x}(t^{n+1})$ as shown in Figure 1a . A algorithm must be used to find the element that the departure node be, then the velocity field in departure node ($\mathbf{v}_d^n$) is calculed by barycenter coordinates interpolation between nodes of element found. As shown in Figure 1b , three situations may occur depending on the trajectory: the first and the second situations are similar, differentiating only the trajectory length. In the first situation, the departure node is inside near element from current node, while the second situation the departure node is inside far element from current node. The third situation, the departure node is outside domain then the vorticity field in departure node receives the boundary condition value of nearest node to departure node.
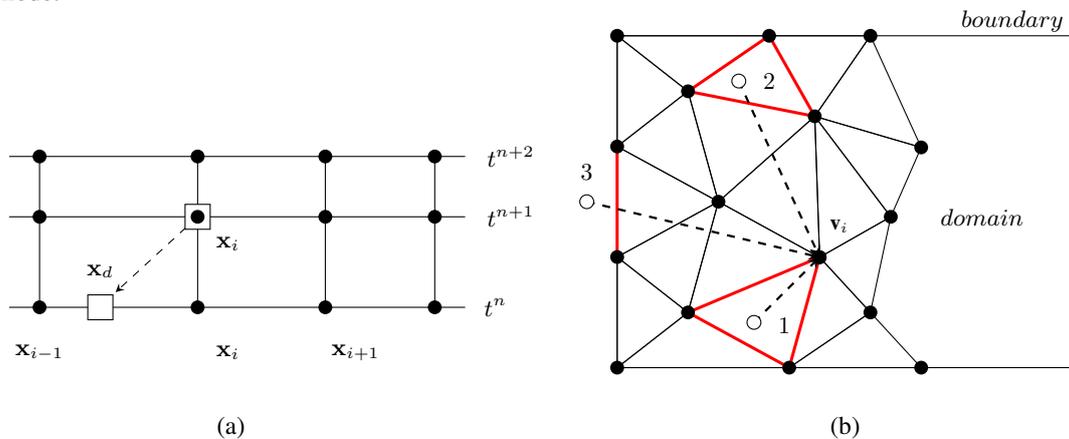

(a) (b)

Figure 1. In (a), an one-dimensional space scheme where the departure node x_d is found by integrating the mesh backward time. In (b), a two-dimensional space scheme where three situations may occur in searching procedure.

The triangular element with linear interpolation was used for the pressure field and a modified cubic element (2D MINI) was used for the velocity field, in order to respect the Babuska-Brezzi restriction (Babuska (1971) and Brezzi

(1974)). These elements consists in three nodes in the vertices and one node in the baricentric for MINI element case. The elementary matrices of this element are calculated using the Gaussian Quadrature, whose parameters can be found in the literature Cowper (1973). These elements are represented by:
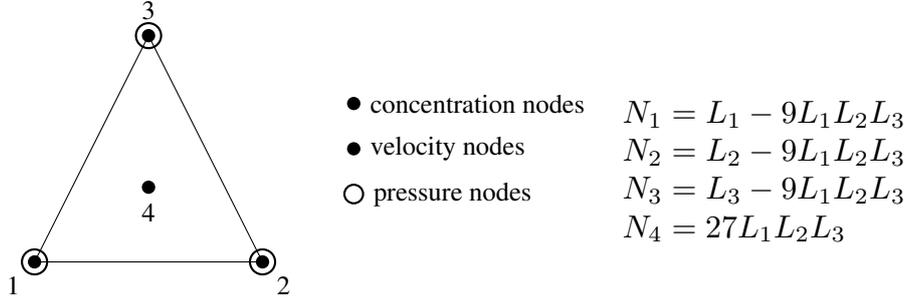

$$N_1 = L_1 - 9L_1 L_2 L_3$$
$$N_2 = L_2 - 9L_1 L_2 L_3$$
$$N_3 = L_3 - 9L_1 L_2 L_3$$
$$N_4 = 27L_1 L_2 L_3$$

● concentration nodes
● velocity nodes
○ pressure nodes

Figure 2. The linear triangle finite element for pressure field and the MINI element for velocity and concentration fields. The L_1, L_2 and L_3 are the linear combination of the triangle area coordinates and N_1, N_2, N_3 and N_4 are the resulting shape functions.

where, a linear combination of the area coordinates L_1, L_2 and L_3 generates the shape functions N_1 to N_4. The pressure p field is evaluated and computed at vertice nodes, while the velocity **v** and concentration e fields are evaluated and computed at all nodes. Thus, we present the final version of the discrete matrix form of the dimensionless governing equations used in this work:

$$
\begin{bmatrix} \frac{M}{\Delta t} + \frac{1}{Re}\left(K + 2M_{1/r}\right) & & -G_r \\ & \frac{M}{\Delta t} + \frac{1}{Re}K & -G_z \\ D_r & D_z + M_{1/r} & 0 \end{bmatrix}
\begin{bmatrix} V_r^{n+1} \\ V_z^{n+1} \\ p \end{bmatrix}
=
\begin{bmatrix} \frac{M}{\Delta t} V_{rd}^n \\ \frac{M}{\Delta t} V_{zd}^n \\ 0 \end{bmatrix}
+ bc
$$

$$
\left[\frac{M}{\Delta t} + \frac{K}{ReSc}\right] e_i^{n+1} = \frac{M}{\Delta t} e_d^n + bc_e
$$

The direct solution of these equations results in the computation of the velocity **v**, pressure p and the drug concentration e at all mesh nodes.

3. RESULTS AND DISCUSSION

The dynamics of drug concentration diffusion in a coronary artery with drug-eluting stent was investigated in a complex geometries using an Eulerian 2D-Axisymmetric approach. That is, the coronary artery was approximated as an axisymmetric plannar domain. Therefore, only half domain was simulated. The blood was modeled as single-phase, incompressible and Newtonian fluid, the diffusion coefficient was considered as constant. The lumen radius of the coronary artery used was R = 0.0015 m, the viscosity used was $\mu = 0.0035$ N.s/m^2 and the density used was $\rho = 1060$ kg/m^3 as suggested by Bozsak *et al.* (2014). According to Kessler *et al.* (1998), the blood velocity in the coronary artery is $u = 0.12$ m/s, thus resulting in the Reynolds number based on the channel's radius of $Re = 54.5$.

The solution of dynamics of drug concentration in a coronary artery with drug-eluting stent was simulated using a complex geometries. The lumen radius was used as characteristic length; therefore, all geometry parameters will be presented as a lumen radius function. Thus, the width between the symmetric axis (bottom line) and the wall (top line) was equal to R = 1 (nondimensional value). The length of channel, that is, the difference between the inflow (left line) and the outflow (right line) was equal to L = 10 R. Initially, the 2-norm relative error of the tangential velocity component is presented and it is compared with the first and second order convergence curves. To obtain the tangential velocity, the Straight Channel was used, where the geometry is represented by figure 3a. Then, the complex geometry used to analyse of dynamics of drug concentration in a coronary artery is called the *Curved Channel with Stent* and it is represented by Figure 3b. This geometry is a model of coronary artery. This simplified model does not require a image processing; therefore, the mathematical equation use to describe the curve is sufficient. The width and length of this geometry is similar to Straight Channel. However, the drug-eluting stent of length equal to 6.55 R was modeled in this geometry by 10 uniform spaced semi-circles with radius equal to 0.125 R. An atherosclerosis was considered for this case, where a sinusoidal equation was used to model 40% of channel obstruction. The concentration diffusion was investigated using two drug types, whose *Schmidt numbers Sc* were: $Sc = \{10, 100\}$, which are equivalent to drug-lumen mass diffusion rates of $D = \{30, 330\} \times$

10^{-6} m^2/s respectively. The simulation was visualized using the *Paraview* open-source software proposed by Henderson (2007) Henderson (2007).

(a) Straight Channel
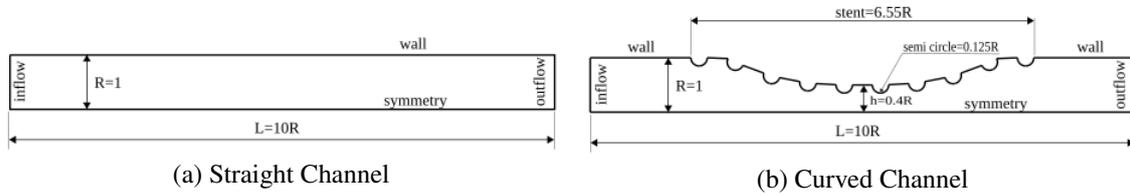

(b) Curved Channel

Figure 3. Nondimensional domains for the dynamics analysis of concentration diffusion in coronary artery with drug-eluting stent. The lumen dimensionless width used was R = 1 and the lumen length was L = 10 R for the (**a** and **b**) cases. The drug-eluting stent of length equal to 6.55 R was modeled for these geometries by 10 uniform spaced semi-circles with radius equal to 0.125 R. For (**a**) geometry, the straight channel was considered, where the atherosclerosis were not present. However, an atherosclerosis was considered for (**b**) case, where a sinusoidal equation was used to model 40% of channel obstruction.

3.1 Straight channel

The figure 4 shows the 2-norm relative error between the numerical solution and the analytical solution for tangential velocity component, using several unstructured triangular meshes with cubic interpolation, ranging from 100 to 7000 elements. Moreover, the relative error is compared with the first and second order convergence curves on a log-log scale. It was simulated for four unstrutuced meshes, that are: 100, 400, 1600 and 6400 elements and the 2-norm relative error for each mesh were, respectively, 12.00%, 2.98%, 0.97% and 0.25%. As can be seen, the 2-norm relative error of the numerical solution for Straight Channel flow has the form of first order convergence. Thus, when increasing the number of elements, the relative error of the numerical solution regresses linearly.
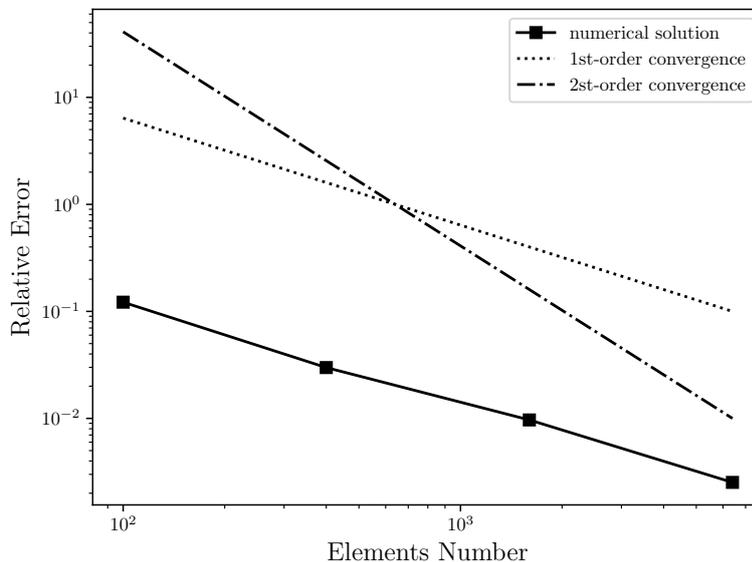

Figure 4. Convergence order for the tangential velocity in log-log scale: It is estimated that the 2-norm relative error of numerical solution has first order convergence.

The figure 5 presents the spatial and temporal distribution of the blood tangential (left column) and radial (right column) velocities for several time steps. The red color refers the maximum value and the blue color refers the minimum value. It is possible observed that the maximum tangential velocity is localized in the symmetric axis. Whereas the radial velocity component has zero value. The maximum dimensionless tangential velocity for the Straight Channel is $V_z = 2.0$. Conveting to dimensional values, the maximum tangential velocity assumes $V_z = 24.0 cm/s$, that is, more than 2 times the average blood velocity in coronary artery. However, this difference was expected because the tangential velocity profile is a parabola curve, ranging zero to 2.0.
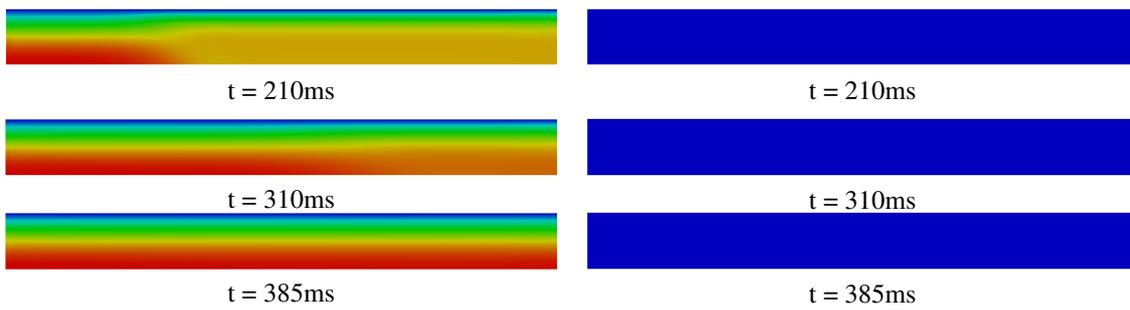
Figure 5. The spatial and temporal distribution of the blood tangential (left column) and radial (right column) velocities for several time steps. The red color refers the maximum value and the blue color refers the minimum value. The maximum dimensionless tangential velocity for the Straight Channel is more than 2 times the nominal blood velocity in coronary artery. However, the difference was expected due to the parabola profile the tangential velocity of the blood flow. Whereas, the radial velocity assumes the zero value in all channel.

3.2 Curved channel with stent

In this section, will be present the simulation of dynamics of drug concentration in a coronary artery with drug-eluting stent. The complex geometry used to model the coronary artery was called the *Curved Channel with Stent* and it is represented by Figure 3b. This simplified model does not require a image processing; therefore, the mathematical equation use to describe the curve is sufficient. The width and length of this geometry is similar to Straight Channel. However, the drug-eluting stent of length equal to 6.55 R was modeled in this geometry by 10 uniform spaced semi-circles with radius equal to 0.125 R. An atherosclerosis was considered for this case, where a sinusoidal equation was used to model 40% of channel obstruction. The domain was discretized using 1887 elements.

The figure 6 shows the comparison between the steady state tangential velocity profile in the middle section channel, that is, $z = 5.0R$ for the Straight Channel and Curved Channel with Stent. As expected, the maximum tangential velocity tends to symmetric axis as the Straight Channel. Moreover, it is possible to observe an inversion of the velocity field sense at the top of the figure. This inversion occurs in the region that is located between the stents strut semi-circles. It is also possible to observe that the maximum tangential velocity field in curvel channel reaches the $V_z = 4.5$ non-dimensional value, that is, more than 4 times the blood velocity in coronary artery without atherosclerosis and stent strut placed. This increase can influence the dynamics of blood flow and its biological processes and a more detailed analysis should be performed.
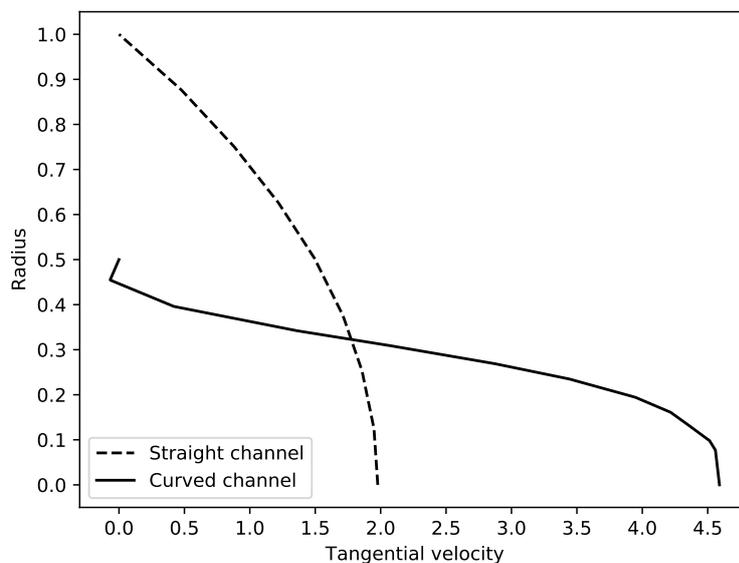

Figure 6. The comparison between the steady state tangential velocity profile in the middle ($z = 5.0R$) of the straight channel and curved channel with drug-eluting stent. As can be seen, the maximum tangential velocity is the symmetric axis. However, in the curved channel with stent reaches the 4.5 non-dimensional value, whereas the straight channel reaches the 2.0.

Figure 7 presents the spatial and temporal distribution of the blood tangential (left column) and radial (right column) velocities for several time steps. The red color refers the maximum value and the blue color refers the minimum value. It is possible observed that the maximum tangential velocity is localized in the maximum obstrution of channel, due to the atherosclerosis. Whereas for the radial velocity component, the drug-eluting stent implantation makes the blood is initially directed downwards and changes the direction close to the end of channel. The maximum dimensionless tangential velocity for the Curved Channel with Stent is $V_z = 4.5$. Conveting to dimensional values, the maximum tangential velocity assumes $V_z = 54.0cm/s$, that is, more than 4 times the blood velocity in coronary artery without atherosclerosis and drug-eluting stent implanted. This increase can influence the dynamics of blood flow and its biological processes; therefore, a more detailed analysis should be performed. In addition, it is also possible to observe an inversion of the tangential velocity field direction at the top of the figure. This inversion occurs in the region that is located between the stents strut semi-circles and a possible coagulation should be checked.

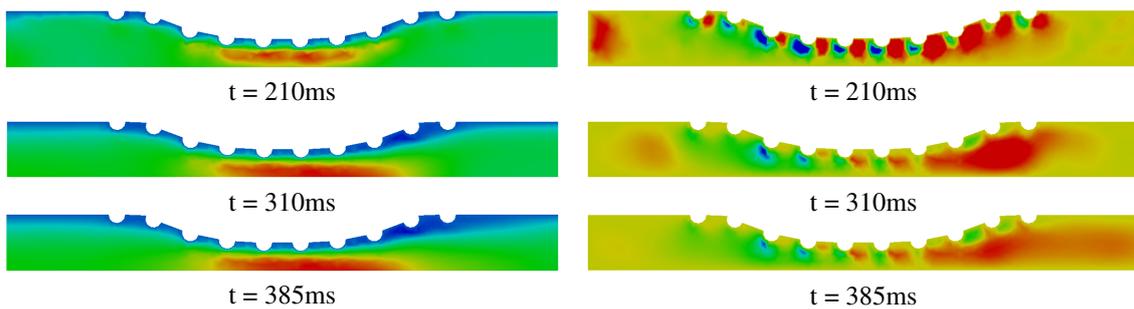| t = 210ms | t = 210ms |
| t = 310ms | t = 310ms |
| t = 385ms | t = 385ms |

Figure 7. The spatial and temporal distribution of the blood tangential (left column) and radial (right column) velocities for several time steps. The red color refers the maximum value and the blue color refers the minimum value. The maximum dimensionless tangential velocity for the Curved Channel with Stent is more than 4 times the blood velocity in coronary artery without atherosclerosis and drug-eluting stent implanted.

The figure 8 presents the spatial and temporal distribution of the pressure field (left column) and streamlines (right column) for several time steps. For the pressure field simulation, the null value was set in the outflow boundary (right line in the domain). The red color refers the maximum value and the blue color refers the minimum value. It is possible to observe a decrease value close to central channel. This decrease region causes a recirculation phenomena and a possible coagulation should be checked. Morever, the recirculation zones can be better seen in the streamlines of the bloodstream (right column).

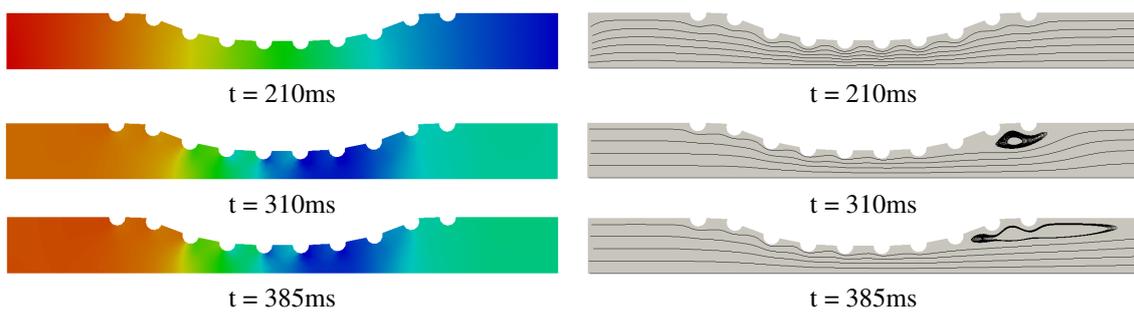| t = 210ms | t = 210ms |
| t = 310ms | t = 310ms |
| t = 385ms | t = 385ms |

Figure 8. The spatial and temporal distribution of the pressure field (left column) and the streamlines of the blood flow (right column). It is possible observed a recirculation zones after the stent strut. A possible coagulation should be checked.

The figure 9 presents the spatial and temporal distribution of the concentration for $Sc = 10$ (left column) and $Sc = 100$ (right column) fields for several time steps. The red color refers the maximum value and the blue color refers the minimum value. For the concentration field, the red color represents 100% and the blue color represents 0% of the diffused concentration in the bloodstream. Is possible to observe that the concentration diffusion acquires the steady state about 210 milliseconds. In addition, a large portion of the diffused drug in bloodstream is quickly spread and the concentration field is more dispersed at the end of the channel due to the direction of the blood flow. For comparison between the two Schmidt numbers simulated, the diffusion of the $Sc = 100$ is slower, as was expected. This diffusion affects the density and viscosity of the blood and consequently the Reynolds number is changed. Therefore, the velocity field would also be affected. However, this influence is not considered in this work.

t = 210ms   t = 210ms

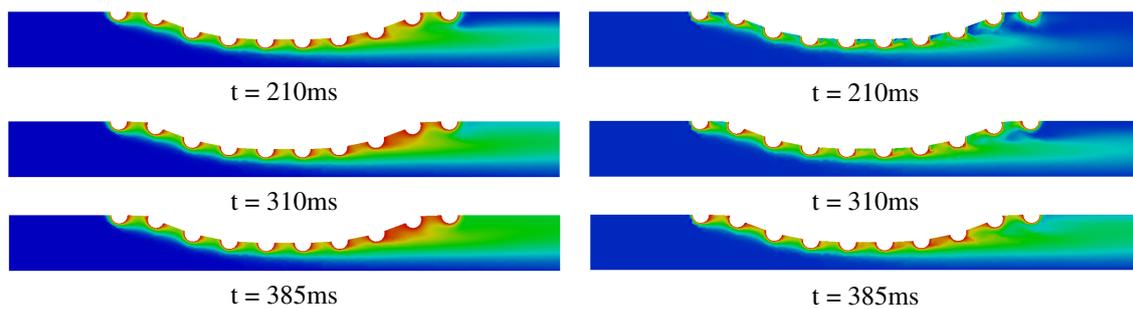t = 310ms   t = 310ms

t = 385ms   t = 385ms

Figure 9. The spatial and temporal distribution of the concentration diffusion using the $Sc = 10$ and $Sc = 100$ drug coefficients for the Curved channel with the drug-eluting stent. Is possible to observe that the concentration diffusion acquires the steady state about 210 milliseconds. A large portion of the diffused drug in bloodstream is quickly spread and the concentration field is more dispersed at the end of the channel due to the direction of the blood flow. This diffusion affects the density and viscosity of the blood. Therefore, the velocity field would also be affected.

4. CONCLUSION

In this work, the finite element code for 2D Axisymmetric Navier-Stokes with species transport equation using semi-Lagrangian scheme was developed to compute biological flows found in coronary artery diseases was performed. The dynamics of concentration diffusion in coronary arteries requires a robust numerical method to compute the solution of the differential equations in a relevant model specially due to the presence of the thin drug concentration boundary layer that must be accurately captured. According to the results presented in the Straight Channel, the numerical code developed proved to be able to perform simulations in complex geometries such as those found in problems involving cardiovascular diseases.

Recirculation zones were observed between the stents strut semi-circles and substantially increasing of velocity in arteries with atherosclerosis of more than four times if compared to a health artery. This increase influences the dynamics of blood flow and its biological processes. Moreover, the drug-eluting concentration in bloodstream is more dispersed at the end of the curved channel due to the direction of the blood flow and this diffusion affects the density and viscosity of the blood and consequently the Reynolds number. It was observed that the flow and drug spatial distributions before the fat buildup was not affected by the atherosclerosis. However, the tests present a strong influence of the geometry of the channels on the drug accumulation after the buildup for cases with $Sc = 10$ and 100. In addition, the Schmidt number directly influences the drug transport in the blood flow, where the transport of chemical species becomes purely convective when low mass diffusivity coefficients are used; therefore, the choice of the drug plays an important role in the bloodstream diffusion. Drugs with low mass diffusivity coefficients should be taken into account at drug-eluting stent design, in order to decrease the chemical species dissolution in the bloodstream. However, the efficiency of these drug-eluting stents in the artery coronary wall should be investigated.

5. ACKNOWLEDGEMENTS

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