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SELECTION AND VALIDATION OF A TURBULENCE MODEL FOR THE NUMERICAL SIMULATION OF THE FLOW AT HEMODIALYSIS CANNULAS

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Abstract. *In recent years, CFD has become an increasingly used tool in the design of blood-based devices. Particularly, the estimation of red blood cell damage (hemolysis) becomes an important challenge to CFD scientists since the blood is a complex fluid present in turbulent regime in most pumping devices. Moreover, previous CFD studies on blood hemolysis lack of reliable relationships between hydraulic results and hematological responses. The objective of this work is to foresee a methodology for performing realistic CFD simulations that lead to reliable hydraulic and hematological correspondence. Cannulae geometries were studied to numerically assess a relatively simple flow with documented hematological data. For the turbulence modeling, a direct numerical simulation (DNS) for a coaxial jet array was used as a benchmark for the selection of an appropriate turbulence model, since the Cannulae approximates the coaxial jet features. Velocity and stress time-averaged profiles were compared between DNS results and the turbulence models. These results, pointed to the Shear Stress Transport with Gamma Theta correlation for transition model as the optimum turbulence model in that geometry. Accurate and reliable hydrodynamic CFD results were obtained for the Cannulae as a previous step to further hematological calculations with a minimum degree of uncertainty.*

1 INTRODUCTION

When blood enters in contact with a non-biological environment, several issues may arise. Osmotic and thermal effects, chemical processes, or even the wall contact could lead to damage of blood cells. But the most relevant source of blood damage usually comes from shear stresses. Under certain conditions, these stresses will provoke the rupture of the membrane of red blood cells, and the subsequent release of hemoglobin into plasma, which is called hemolysis.

The study of this phenomenon is primordial in the design of biomedical devices, such as blood pumps, dialysis machines, heart valves, catheters and cannulas, among others. The in-vitro evaluation of these devices is the most reliable way to perform the hematologic study [1]. However, it requires great number of repetitions, due to statistical variations, to assure the validity of the results. These experiments are quite expensive, increasing the design and development cost of the blood-based medical devices.

As a result, the hemolysis analysis by means of computational fluid dynamics (CFD) appears as an attractive alternative [2,3], because it could decrease the cost and time of design and development of medical devices. With CFD analyses, accurate calculation of hydrodynamic variables, such as velocity, pressure and stress fields could be obtained for the devices under study. Through a hemolysis model, a relationship between these hydraulic results and the corresponding hemolytic response could be calculated. Nevertheless, a reliable and validated general hemolysis model does not exist up till now. So far, the data obtained for hemolysis at one-dimensional stress experiments has been correlated by means of a multi-variable regression in terms of shear stress and exposure time [4], but consensus about a methodology for the application of such correlations to CFD results has not been established yet.

For evaluation of reliability and accuracy of hemolysys models, it is advisable to progressively test complex geometries. The cannulas [5,6], which were studied in this work, and capillaries [7], are the simplest geometries of biomedical devices for which experimental measurements of hemolysis are available.

2 HEMOLYSIS CALCULATION AND ESTIMATION

As mentioned before, the most popular hemolysis model, the Giersiepen-Wurzinger equation, is based on a multi-variable regression over experimental data obtained from a one-dimensional stress case [4]. The equation has the following form:

$$\frac{\Delta PfHb}{Hb} = \left(3.62 \times 10^{-7}\right)\tau^{2.416} t^{0.785} \tag{1}$$

where $\Delta PfHb$ is the change on the plasma free-hemoglobin, Hb is the total amount of hemoglobin in the blood sample, τ is the constant shear stress which the blood sample undergoes and t is the exposure time to that stress.

Several methods have been proposed for the calculation of hemolysis departing from Eqn. (1). Integration of the equation along streamlines is certainly the most popular [6,8]. Other authors propose a Lagrangian technique of particle seeding [9], and tracking the evolution of the hemolysis on individual particles. The accuracy of both methods is related with the accuracy of CFD results, and the number of streamlines or particles. Recently, an Eulerian approach has been proposed [10,11], based on a transport equation derived directly from Eqn. (1) and ASTM standards [1].

3 TURBULENCE MODELING

Even though the experimental setup of Wurzinger [4] only evaluates the laminar regime, other authors [7] have proved numerically and empirically the remarkable effect of turbulent stresses over hemolysis. This is an important subject of study, because in most of the biomedical devices, and particularly in blood pumps, the flow regime is predominantly turbulent.

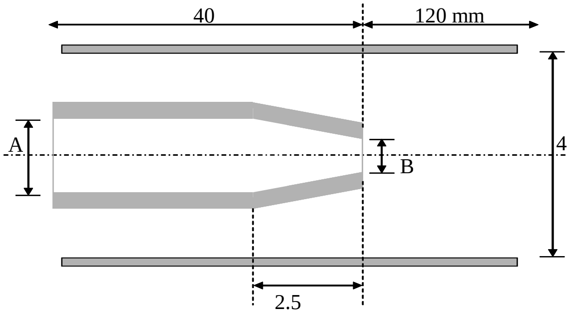

Figure 1: Dimensions of cannulas studied by De Wachter & Verdonck

De Wachter and Verdonck [5,6] studied empirically and numerically the hemolysis in cannulaes during a dialysis procedure. Figure 1 describes the geometry used in the numerical study. The inner diameters A and B stand for the cannulae core and its tapered end, respectively. The dimensions of the different sizes of cannulas studied are listed in Table 1.

Table 1: Dimensions of the cannulas in Figure 1

	A (mm)	B (mm)
13G	2.21	1.6
14G	1.91	1.3
16G	1.45	1.2

De Wachter and Verdonck specified an operational range of blood flow through the cannulas in dialysis procedure, with a maximum of about 400 ml/min, and a physiological range of blood flow through the arteries between 500 and 1200 ml/min. Figure 2 details the different regions inside the vessel and around the cannulae. The Annular region corresponds to the zone bounded by the blood vessel wall and the outer wall of the cannulae. The Cannulae region, as its name indicates, is bounded by the cannulae. The vessel region is neither cannulae nor annular, and it's bounded by the blood vessel. Taking the maximum value of flow ranges, the average Reynolds number for each region can be calculated. The results are reported in Table 2.

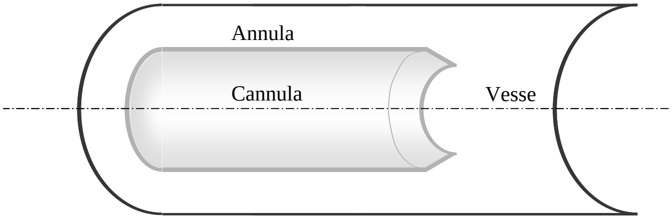

Figure 2: Regions of the domain studied by De Wachter and Verdonck

Table 2: Average Reynolds number per region at maximum flow rate for different cannulas

	Annular	Cannulae	Vessel
13G	1158	1680	2783
14G	1215	1943	2783
16G	2559	1314	2783

Reynolds number above 2300 ~ 2500 are a signal of the existence of a turbulent regime in that region. Therefore, those Reynolds numbers indicate that transition form laminar to turbulent regime may occur within the domain under study. This transition was not considered in the previous numerical work by De Wachter and Verdonck [6], where they solved the laminar Navier-Stokes equations.

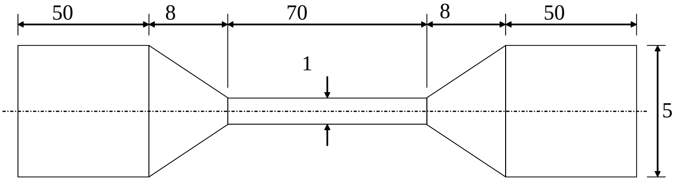

Figure 3: Dimension of the capillary studied by Antaki et al.

On the other hand, Kameneva et al. [7] have studied numerically and experimentally the blood capillary described in Figure 3. They analyzed both laminar and turbulent regimes, showing a prominent effect of turbulence onto hemolysis rate. Therefore, and accurate modeling of the turbulence its highly relevant, due to the high amount of uncertainty added to the flow solutions by the selection of different turbulence models

4 TURBULENCE BENCHMARK

Based on the geometrical characteristic of cannulas and the capillary, a benchmark to validate the selection of the turbulence model has been selected. Balarac and Métais [12] performed a Direct Numerical Simulation (DNS) for an array of coaxial jets, which resemble very closely the characteristics of the flow, as it can be seen in Fig. 4. In both cases, there is a shear layer between the inner and outer streams. The capillary could be considered as a particular case of the jet (especially at the diverging cone), where both annular and central velocity are alike.

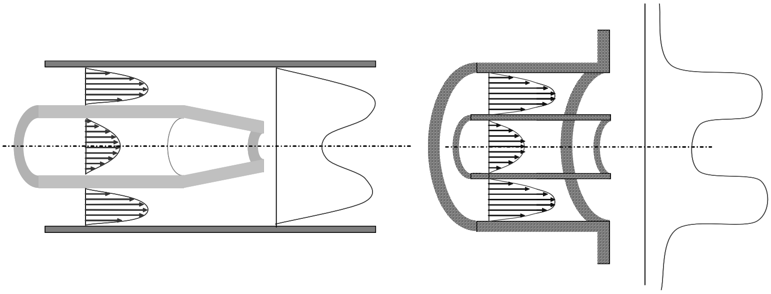

Figure 4: Similitude in the flow at cannulae (left) and at the array of coaxial jets (right)

5 NUMERICAL RESULTS

Hydrodynamic results of jets array studied by Balarac and Métais were obtained with a commercial 3D finite volume code (ANSYS CFX). This code uses finite volume for the discretization of the incompressible Reynolds-Averaged Navier-Stokes (RANS) equations. For closure, the set of differential equations corresponding to the turbulence model is solved within the preceding numerical system. By comparison between the DNS velocity profiles and the corresponding from the RANS simulation, the best suitable turbulence model was selected. The velocity at centerline of the jets, and the radius of the jet were the comparison variables.

Figure 5 shows the structure of the numerical domain used for the solution of the RANS equations. The domain was discretized with a non-uniform hexahedral mesh. The hexahedral grid takes advantage of the polar symmetry of the jet array, working only with one-quarter of the domain. Table 3 presents the number of control volumes on each grid used in the refinement study. The boundary conditions for the RANS simulations were set to mimic those from the DNS simulations: a laminar inlet profile, as shown in Fig. 5.

The centerline velocity and the jet radius "δelta" were calculated for each grid, with a standard k-ε turbulence model. The results are plotted in Fig. 6. As it can be seen, the curves are almost congruent, a signal of a sufficiently refined grid. The following calculations were all performed using the n44_87 grid. Figure 7 shows the results with different turbulence models.

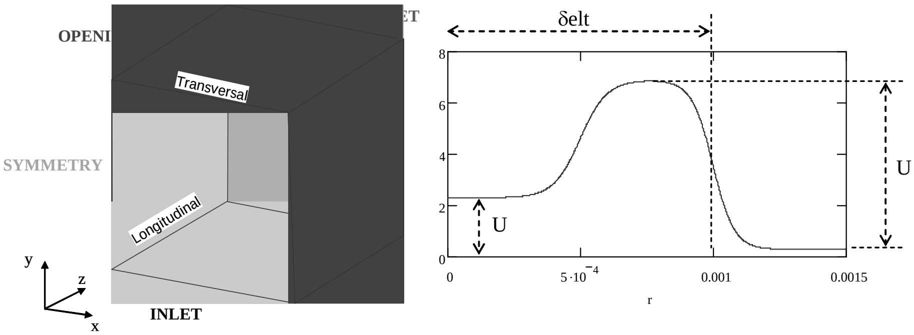

Figure 5: Numerical domain used at the RANS solution of the coaxial jets array (left), laminar inlet profile used in this domain (right)

Table 3: Grids size for the refinement study of coaxial jets

Grid	Transversal Nodes	Longitudinal Nodes	Total Control Volumes
n22_44	22	44	18 963
n28_55	28	55	39 366
n35_69	35	69	78 608
n44_87	44	87	159 014

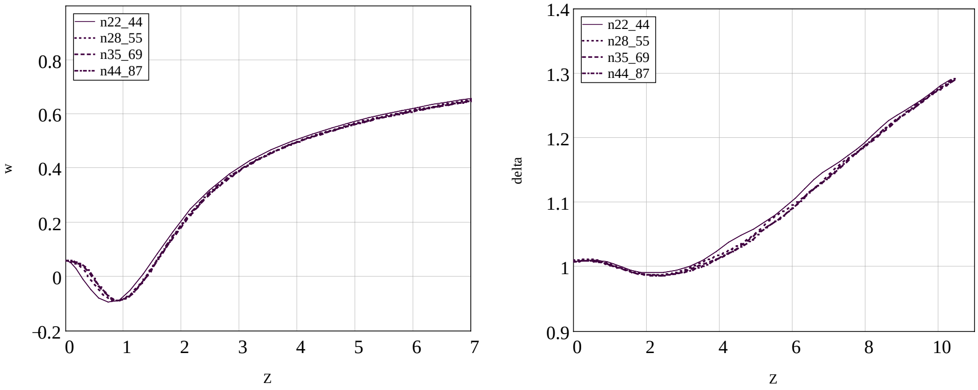

Figure 6: Results of refinement study for coaxial jets: centerline velocity (left) and jet radius (right) as a function of the axial coordinate Z

6 DISCUSSION AND CONCLUSIONS

Different turbulence models (k-ε, k-ω, SST and SST with transitional turbulence) were found to significantly differ in predicting the flow development and the laminar to turbulence transition. Among the considered models, the one that better resembles the behavior of the jets DNS benchmark is the SST with transitional turbulence, as it can be seen in Fig. 7. The SST transitional model accurately predicts the development and transition of the flow from laminar to turbulent regime. Therefore, this should be the choice for the simulation of cannulas, capillaries and other geometrically similar biomedical devices, where the turbulent regime is present.

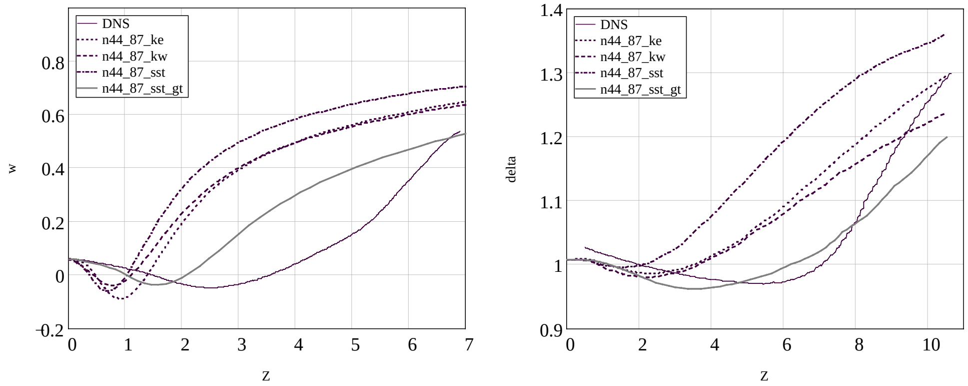

Figure 7: Results with different turbulence models: centerline velocity (left) and jet radius (right) as a function of the axial coordinate Z

In this work, a simple validation procedure for a turbulence model to be used in cannulas and capillaries were developed. The accurate calculation of the turbulent stress becomes mandatory, especially when they have a predominant role at the numerical estimation of blood damage inside these biomedical devices. The use of a validated turbulence model diminishes the amount of uncertainty inherent to numerical blood-damage estimation. Further investigation into the hemolysis model and the comparison of the numerical result of different models with experimental values of hemolysis are currently under way.

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