Modeling Hemodynamics with Abaqus/CFD Steady State Solver: FDA Benchmark Nozzle Model

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***Abstract**: Understanding the blood flow dynamics (hemodynamics) and the fluid forces exerted on the blood by implantable medical devices and predicting blood damage is an intricate part of interventional medical device design. Computational techniques such as Computational Fluid Dynamics (CFD) are increasingly being used as a tool for describing complex hemodynamics and calculating the fluid forces such as pressure and shear stress. However, this technique is challenged by the lack of standardized methods for validation and verification of the results.*

In an effort to standardize the process, the FDA made an initiative in 2008 to engage the Medical Device/CFD Community worldwide to participate in an open challenge that involves CFD computation of blood flow and its experimental validation with Particle Image Velocimetry (PIV) on a benchmark nozzle model. The goal of the CFD phase of the study was to understand the limitations of CFD, understand the variability that arises due to choice of software or solver, and the influence of user expertise level and diverse modeling and meshing techniques. This information would then be employed to identify best practices and define the critical techniques necessary to achieve credible results. Though a variety of software packages have been used by 28 different groups from 6 countries, Abaqus/CFD has not been publicly applied in this challenge.

In this study we aim to assess the performance of Abaqus/CFD in modeling hemodynamics using the FDA Benchmark Nozzle model. The Nozzle model consists of a tube with a straight section, followed by a conical section, a section with reduced tube diameter and a section with a sudden expansion in tube diameter. The device was designed to include accelerating flow, decelerating flow, variations in shear stress and velocities, and recirculating flow, all of which may be present in a medical device and relate to blood damage. Five different flow rates corresponding to fully laminar, transitional and fully turbulent flow were modeled with laminar and turbulent solvers. In this study we have used pure hex mesh as well as the steady state solver introduced recently to solve both laminar and turbulent flow problems and compared the results with published experimental data. The hex-dominant mesher available in the 3DExperience platform was also tested with this model (results not presented here). For solving the turbulent flow at higher flow rates we tested three models, namely Spalart-Allmaras, k-ε and k-ω models. Results of interest were the axial velocity, pressure and fluid shear stress along the centerline, axial velocity along a radius of cross section at selected planes, and wall shear stress.

Overall, Abaqus/CFD results were found to match very well with experiment results and faired competently with other software results. The k-ω model was found to perform best among the three turbulent models. This detailed study provides valuable insight into effective strategies for modeling hemodynamics using Abaqus/CFD.

***Keywords**: CFD, hemodynamics, FDA Nozzle, Sudden expansion, steady state solver, turbulent models, Spalart-Allmaras, RNG k-ε model, SST k-ω model*

1. Introduction

Computational Fluid Dynamics (CFD) techniques are intensely used in the design and analysis of components in heavy industries, such as the aerospace and automotive industries. Following the same trend this technology is being used in the medical device industry to design, develop and analyze devices like ventricular assist devices, prosthetic heart valves, stents, blood filters and hemodialysis catheters. However this technique can not only help in the design process of a device but also can predict the change in the hemodynamic environment (i.e., the change blood flow dynamics and/or the fluid forces exerted on the device). This information is crucial as blood flowing through medical devices is subject to hemolysis or thrombosis. Understanding the effect of hemodynamic forces like shear stress and exposure time on hemolysis has been an area of active research focus for the past decade. Though crucial understanding has been achieved and several power law based empirical formulas have been modeled, the use of CFD and blood damage models in predicting medical device safety has not been adequately proven yet. To successfully implement these techniques for medical device design and/or for regulatory reviews a better understanding of the computational model and experimental validation must be achieved and steps towards "standardized" practices should be taken.

With an aim to utilize this technology to its fullest and standardize it, FDA initiated a critical path initiative named as" Computational Fluid Dynamics (CFD)/Blood Damage Project". The initiative consist of two projects , the first one is CFD/PIV analysis of a Nozzle model that represents an idealized medical device geometry and the second one is a CFD/PIV and blood damage experiments on a heart pump model. The goal of the first project, which has been evaluated in this study, was to assess the current state of the art in CFD analysis in modeling hemodynamics. The experimental PIV analysis was performed in 4 labs, 3 from University research groups and one from the FDA. The averaged data was used for validation purposes. Twenty eight groups from 8 countries participated in the CFD challenge and submitted their simulation results. This project was initiated in 2008 and the experimental results were published in 2010 (Hariharan, 2010). The computational results with experimental validation were published in 2011(Stewart, 2011).

Abaqus/CFD, being a relatively recent addition to the SIMULIA brand has not been documented in this challenge. Therefore the need to validate the standard hemodynamics process and assess the performance of Abaqus/CFD was the prime motivation for this study. The easy accessibility of the experimental results from the FDA repository is an additional reason for choosing this benchmark model as a validation standard.

The FDA Nozzle model consists of a straight tube, a conical section that connects to a straight throat region of smaller diameter, and a sudden expansion region where the diameter suddenly increases back to the original tube diameter. The device was designed to include accelerating flow, decelerating flow, sudden expansion/gradual diffusion, variations in shear stress and velocities, and recirculating flow, all of which may be related to blood damage in medical devices. For this geometry, flow in one direction is a sudden expansion problem, whereas flow in the opposite direction is a conical diffusor problem. In this study we concentrated on the sudden expansion problem. The model was simulated with 5 different flow rates that cover the range of fully laminar to fully turbulent flow.

Through this study we present the capabilities of Abaqus/CFD as a comprehensive tool offered by SIMULIA, capable of solving for laminar, transitional and turbulent flow with accuracy. Abaqus/CFD can be used within the Abaqus/CAE environment in all three stages of analysis - modeling/meshing, solving and post-processing. In version 6.13, Abaqus/CFD has introduced a steady state solver that is robust and uses a 2nd order accurate SIMPLE based algorithm. Abaqus/CFD has also introduced three turbulent flow models, the first one is a one equation Spalart-Allmaras model, and the other two are two equation RNG k-ε and SST k-ω models. The first two models are available in CAE and the last one is available through insertion in the input deck. Details of the modeling technique followed are discussed in the method section, and the simulation results are presented in the Results and Discussion section.

2. Methods

2.1 Nozzle Geometry

The dimensions of the nozzle geometry were obtained from the published literature (Stewart, 2011). The FDA Nozzle model consists of a straight tube of diameter (D) 12 mm, a conical section that reduces the tube diameter to 4 mm in the throat region, and a small straight throat section of 40 mm length which is followed by a sudden increase in tube diameter (D) to 12 mm. The inlet length and the outlet length were left for the analyst to choose. We have chosen the inlet length to be 10 times D. We have used a parabolic inlet velocity profile therefore larger inlet length was unnecessary. For assessing the outlet length, simulations were performed with different outlet length and the velocity profile at the outlet observed. Our objective was to obtain a parabolic velocity profile at outlet. Results with shorter outlet length resulted in a velocity profile where the peak velocity is eccentric. As the length was increased, the outlet velocity was fully developed and peak velocity was concentric. Depending on this criterion we chose the outlet length to be 60D.

The 3D model of the CFD domain as shown in Figure 1a was developed using the solid modeling features in Abaqus/CAE .

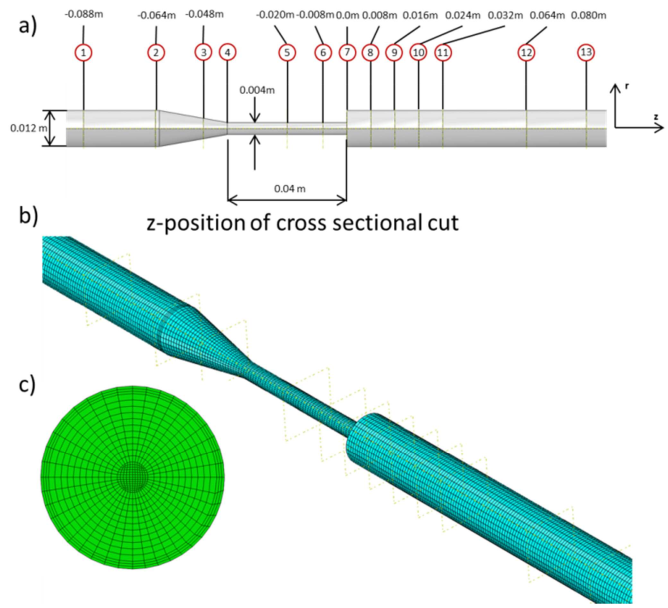


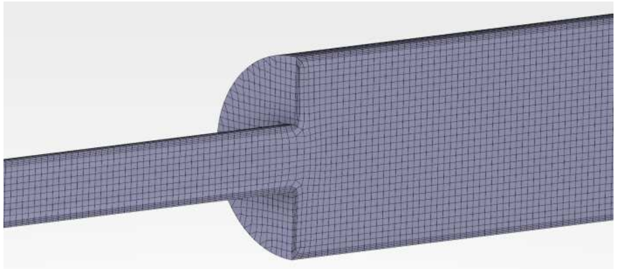
Figure 1. (a) FDA Nozzle model geometry with cross sectional surfaces identified by numbers b) final hex mesh of the model c) view of the radial section of the mesh at inlet

2.2 Meshing

Linear Hex elements were used to mesh nozzle model in this study. The model volume was subdivided along the axial direction and also along the radial direction as shown in in Figure 1b. There were 13 cross sectional surfaces of interest identified for post processing of results that were used for volume subdivision along the axis. The subdivision in the radial direction helped in prescribing adequate seeds near the walls. A mesh refinement was performed by changing the global seed from 0.001 to 0.004 along with adequate seeding of radial and axial edges. The final mesh consists of 1.39 million elements. The final mesh pattern is shown in Figures 1b and 1c.

Another meshing technique was also tested and used for this model. It is the hex-dominant mesher available as part of the R2014 3DExperience platform. It is capable of handling complex geometries in a robust manner, and creating high-quality Hex-dominant 3D meshes. The Hex-dominant 3D mesher includes surface wrapping technology to automatically extract the fluid domain by creating a clean closed 'wetted' surface for subsequent volume meshing. A snapshot of the mesh created for the nozzle geometry is shown in Figure 2 (a). A closer look of the mesh, shown in Figure 2 (b) shows the smooth transition from a finer mesh (near the wall) to a coarser mesh away from the wall. The robustness and the time it takes to create high quality meshes, makes this mesher useful for creating CFD meshes for both simple and highly complex geometries. The results obtained by using this mesh are not included in this paper, but the results were very comparable to the more traditional hexahedral element mesh created using Abaqus/CAE.

(a)



(b)

Figure 2: Nozzle mesh using R2014 3DExperience Mesher

2.3 Materials

Blood is modeled as incompressible fluid with a density of 1056 kg/m^3. It is assumed be a Newtonian fluid with dynamic viscosity of 0.0035 N.s/m^2 as per the guidelines of the challenge (Stewart, 2011)

2.4 Boundary Conditions

Simulations were performed with 5 different inlet velocities ranging from inlet Reynolds number 167 to 2167 as documented in (Stewart, 2011).The flow rates were labeled as Q1, Q2, Q3, Q4 and Q5.The average inlet velocity, flow rate, average velocity at throat and throat Reynolds number are presented in Table 1. Though the inlet Reynolds number indicates the flow to be in a fully laminar zone at Q1 to a transitional zone at Q5, the throat Reynolds number indicates that the flow type ranged from fully laminar at Q1 to fully turbulent at Q5 in the sudden expansion region. In this study we have chosen to represent the flow rate Q1 as fully laminar flow, flow rate Q3 as representative of transitional flow and flow rate Q5 as fully turbulent flow. A parabolic inlet velocity profile $\boldsymbol{V_z}$ was used to model the inlet flow distribution following Equation 1

$$V_z = V_{max}\left(1 - \frac{r^2}{R^2}\right) = \mathrm{a} - \mathrm{b}r^2$$

Equation 1

where $\boldsymbol{V_{max}}$ is 2 times the average inlet velocity, ***r*** is the radial coordinate , ***R*** is the inlet radius and $a = V_{max}$ and $b = V_{max}/R^2$.

The outlet boundary condition was set to zero pressure and a no-slip boundary condition was applied to the wall surface of the model

Table 1. Inlet flow rate, velocity, Reynolds number used in the simulation

	Inlet Re	Average Inlet Velocity	Flow Rate	Peak Velocity (Parabolic)	Parabolic Profile		Velocity at throat	Throat Re
	Re_i	m/s	m^3/s	m/s	a	b	m/s	Re_t
Q1	167	0.05	5.22e-6	0.09	0.09	2563.52	0.42	500
Q2	667	0.18	2.08e-5	0.37	0.37	10234.73	1.66	2000
Q3	1167	0.32	3.65e-5	0.64	0.64	17906.93	2.90	3500
Q4	1667	0.46	5.21e-5	0.92	0.92	25579.14	4.14	5000
Q5	2167	0.60	6.77e-5	1.20	1.20	33251.35	5.39	6500

2.5 Analysis Settings

A steady state incompressible fluid flow analysis was performed in Abaqus/CFD. The steady state method is a new addition to Abaqus/CFD version 6.13 and is based on a second order accurate SIMPLE (Semi-implicit Method for Pressure Linked Equation) based algorithm. Depending on the problem, a proper choice of an under-relaxation factor can significantly increase the convergence rate of the solution. For this study we chose 0.7 for the Momentum equation and 0.3 for the pressure equations and obtained a converged solution in 1000-1500 iterations. For the lowest flow rate Q1 the laminar flow model was used. For all other higher flow rates, we have used the laminar flow model along with three turbulent flow models. Abaqus/CFD offers a Spallart-Allmaras model and RNG k-ε model in CAE and the SST k-ω model can be accessed through the input deck. The Spallart-Allmaras model is a one equation Reynolds Averaged Navier Stokes (RANS) turbulent model that solves for the Reynolds's stress when the Spalart-Allmaras variable kinematic turbulent viscosity is known. Abaqus/CFD recommends calculating the kinematic turbulent viscosity ($\nu^{\sim}$) as 3 to 5 times of the kinematic viscosity (ν) of the fluid. We used a value of 1.3258e-5 Stoke, which is 4 times of kinematic viscosity.

RNG k-ε model and SST k-ω models are two-equation RANS models that solve for Reynold's stress by including two transport equations to represent the turbulent properties of the flow, like turbulent kinetic energy(k) and turbulent dissipation (ε) and /or specific dissipation(ω). The RNG k-ε model is a variant of k-ε models where the Re-Normalization Group (RNG) method is used to re-normalize the Navier stokes equation. The parameters k and ε can be calculated using Equation 2 if the inlet velocity (u_0), turbulent intensity (I) and turbulent length scale (l) is known.

$$k = \frac{3}{2}(u_0 I)^2 \; ; \; \varepsilon = C_\mu^{3/4} \frac{k^{3/2}}{l}$$

Equation 2

C_μ is an empirical constant whose value is 0.085. The SST k-ω model is a two equation eddy viscosity model where a Shear Stress Transport (SST) formulation is combined with a standard k-ω model and represents the "best of both" of the models. The variables for the transport equation are available in Abaqus/CFD whereas the parameters k, and ω can be calculated if the inlet velocity, turbulent length scale and turbulent intensity are known using Equation 3.

$$k = \frac{3}{2}(u_0 I)^2 \; ; \; \omega = \frac{k^{1/2}}{C_\mu^{1/4} l}$$

Equation 3

For this study the turbulent intensity and length scales were not available so we assumed the values to be 0.057 and 0.84 mm, given that turbulence intensity (I) at core of a fully developed pipe flow can be approximated by $I = 0.16 * \mathrm{Re}^{-\frac{1}{8}}$ and the turbulent length scale at inlet can be approximated by 0.07*L, where L is the characteristic length, in this case it is the inlet diameter of the model. Table 2 summarizes the parameter values used for 4 different flow rates (Q2, Q3, Q4 and Q5).

Table 2. Turbulence parameters used for RNG k-ε model and SST k-ω model, for flow rates corresponding to throat Reynolds number

	u_0 (inlet)	k	eps (ε)	omega(ω)	Turbulence Intensity	length scale
Q2:Re = 2000	0.1839	1.64E-04	3.96E-04	28.31	0.057	8.40E-04
Q3:Re = 3500	0.3218	5.04E-04	2.12E-03	49.53	0.057	8.40E-04
Q4:Re = 5000	0.4606	1.03E-03	6.23E-03	70.89	0.057	8.40E-04
Q5:Re = 6500	0.5986	1.74E-03	1.36E-02	92.13	0.057	8.40E-04

Simulations were performed on a desktop computer equipped with an Intel Core™ i7 CPU and 16 GB of RAM. Simulation times were between 5 hours to 12 hours.

3. Results & Discussion

3.1 Centerline Velocity and Pressure

Results were post-processed in the Abaqus/CFD visualization module. Snapshots of the velocity magnitude plot from three different flow rates are shown in Figure 3. The snapshot shows the jet length in the sudden expansion zone for laminar flow model with flowrate Q1 and turbulent flow model with flowrates Q3 and Q5. It should be noted here that there are some instabilities seen for the Laminar case near the outlet. This is an outcome of the steady state plot shown at an instant prior to fully converged solution.

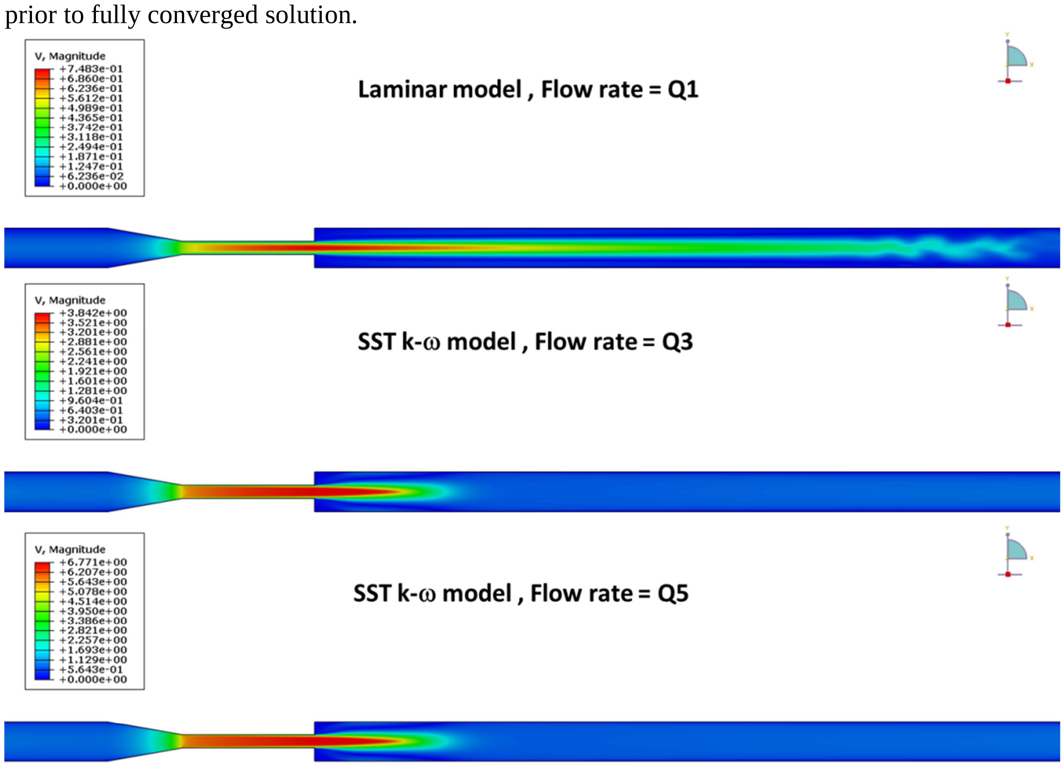


Figure 3 : Velocity magnitude plot obtained from laminar model for flow rate Q1 and turbulent model (SST k-ω model) are plotted for flow rates Q3 and Q5.

A direct comparison of the Abaqus/CFD results with the experimental data obtained from FDA repository is presented in Figure 4.

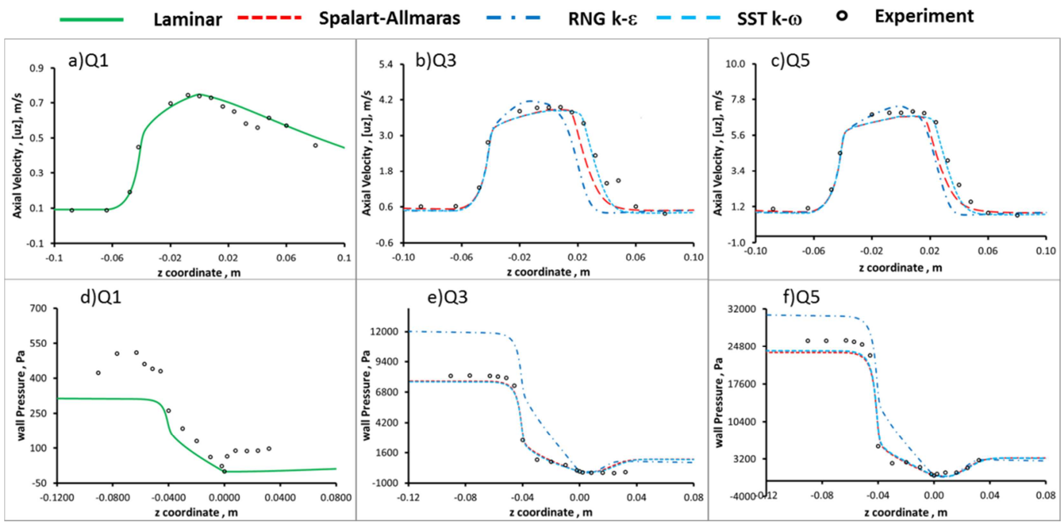


Figure 4 : Centerline velocity in the axial direction, obtained from laminar and turbulent simulations, are plotted for flow rates (a) Q1 , (b) Q3 and (c) Q5. Similarly, wall pressure, represented by the centerline pressure in the axial direction is plotted for flow rates (d) Q1 (e) Q3 and (f) Q5. Flow rates Q1, Q3 and Q5 are representative of fully laminar flow, transitional flow and fully turbulent flow.

Centerline velocity in the axial direction and pressure data were recorded using the ‘path’ feature in the visualization module and plotted in Figure 4. The data obtained were for three different flow rates that are representative of fully laminar (Q1), transitional (Q3) and fully turbulent (Q5) flow types. Due to very little radial pressure gradient, wall pressure is represented by the centerline pressure. The experimental data presented in Figure 4 are an average of 3 different experimental data sets obtained from the FDA repository [3]. The experimental and computational pressure values are referenced with respect to the pressure at the location of the sudden expansion (z=0.0). Our simulation results matched very closely with the experimental data for laminar, transitional and turbulent flow. As the flow through the nozzle before the sudden expansion (z=0) region is truly laminar, the centerline axial velocity characterized by the laminar flow model was in excellent agreement with the experimental data for all three flow rates. Flow beyond the sudden expansion zone is complicated and none of the models were an exact match with the experimental data. Similar behavior was reported by the other contributors to the challenge and this was comprehensively discussed in the FDA publication (Stewart, 2011). At the sudden expansion zone the laminar flow model did well for lower flow rates and demonstrated fluctuations for transitional and fully turbulent flow rates. Here, the SST k-ω model and Spallart-Allmaras model achieved the best agreement with the experimental data.

Figure 4(d-f) represents the pressure plots. Clearly pressure from laminar flow model for flow rate Q1 (Figure 3d) did not match with the experimental data. As reported (Stewart, 2011) results from other computational studies did not match with the experiment either. The errors are attributed to experimental error in pressure measurement, and were partly due to wrong reference scaling and were partly for not using differential pressure transducers and were discussed in the literature (Stewart, 2011). For higher flow rates (Q2 & Q3), the largest discrepancy in pressure was observed for the RNG k-ε model. The discrepancy in the pressure characteristics by the RNG k-ε model can be attributed to its inability to characterize turbulence in multiple different length scales as the eddy viscosity is determined from a single selected turbulence length scale. It is also well known that the RNG k-ε does not perform well for transitional Reynolds number, which we believe is the case in cases Q2 and Q3. In addition, the impact of wall mesh resolution requirement (y^+ near the wall) could also be a contributing factor to the deviation from experimental results. Future work will involve using the newly introduced realizable k-ε turbulence model, which uses a hybrid wall functions approach thereby alleviating the need for creating meshes with specific near wall resolution (any y^+ value near the wall) as opposed to the RNG k-epsilon, which had a stringent near wall mesh requirement (y^+>20 near the wall). Similar behavior of the k-ε model was observed by users of other software as well (Stewart, 2011). Though none of the turbulent flow models were an exact match with the experimental data at each location, the Spalart-Allmaras and SST k-ω models did a superior job in characterizing the axial velocity and pressure before and beyond the sudden expansion zone, whereas the laminar model results deviated slightly in the sudden expansion region. The next section describes the axial velocity profile in the radial direction at specific cross sectional surfaces along the axial length of the model.

3.2 Axial velocity profile at selected cross sections

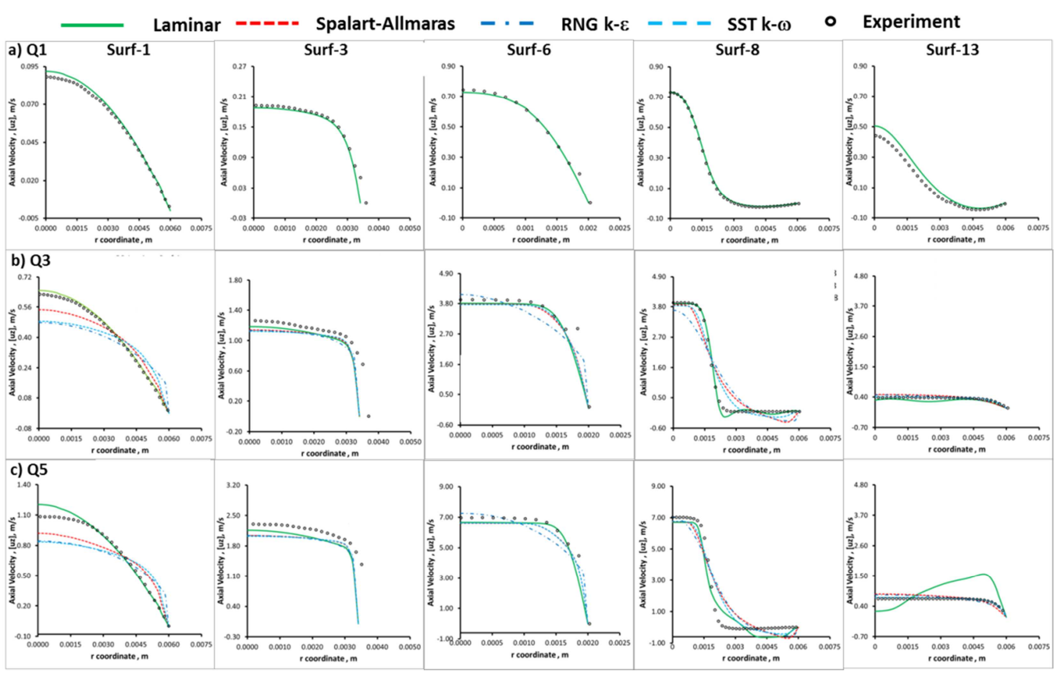


Figure 5 : a) Axial velocity in radial direction at specific cross sectional surfaces (Surf-1,Surf-3,Suf-6,Surf-8 and Surf-13) are obtained from simulation and plotted along each row for three different flow rates (b) Q1 (c) Q3 and (d) Q5.

The nozzle model was subdivided in such a way that 13 cross sectional surfaces were created as shown in Figure 1a. Out of the 13 surfaces, results from only the following surfaces of interest were presented in this study: Surf-1 is closest to inlet, Surf-3 is at the conical section, Surf-6 is at the throat region, Surf-8 is in the sudden expansion zone and Surf 13 is the farthest away from the sudden expansion region. Axial velocities along the radial direction at these cross-sections were recorded for three strategic flow rates (Q1,Q3 and Q5) and presented in Figure 5 (a, b and c) respectively. The experimental data presented here is from one set of experiments obtained from the FDA repository [3] that best matches the average experimental data. As expected, the velocity profile from the laminar flow model matched very well before the sudden expansion zone for all three flow rates. As flow rate increases, the turbulent flow models did a better job in matching the experiment results at and beyond the sudden expansion region, as demonstrated clearly by the Surf-13 results described in Figure 5b and Figure 5c.

3.3 Radial shear rate profile at selected cross sections

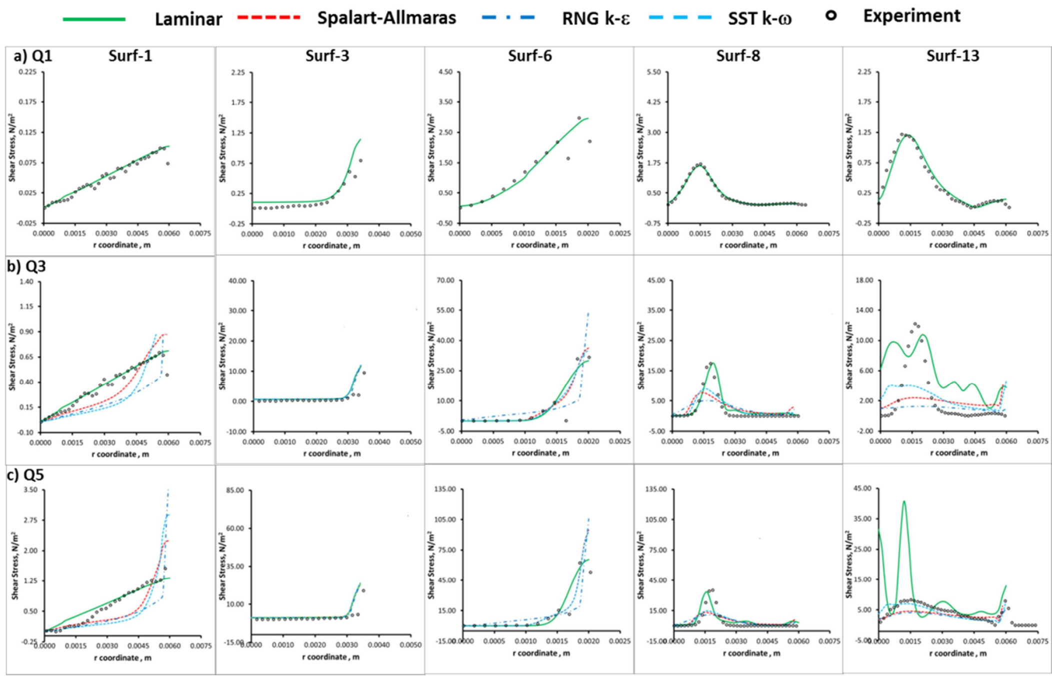


Figure 6 : Shear Rate in radial direction at specific cross sectional surfaces (Surf-1, Surf-3, Suf-6, Surf-8 and Surf-13), obtained from simulation and plotted along each row for three different flow rates (b) Q1 (c) Q3 and (d) Q5.

We have further post processed hemodynamic parameters such as shear rate at selected cross sectional surfaces (Figure 6). Shear Rate is the ratio of velocity and distance and fluid shear stress can be calculated by multiplying shear rate and dynamic viscosity. Results from the laminar flow models matched the shear rate characteristics very well for lower flow rate Q1 and transitional flow rate Q3. With flow rate Q3, a larger discrepancy in shear rate was observed at Surface 10 and none of the models were effective in capturing the true behavior of the flow observed through experiment. However, as the flow rate increased to Q5, the turbulent flow models were successful in capturing the flow behavior at this location. As flow rate Q5 is still in a transitional zone in the inlet tube, the laminar flow model did a better job in capturing the flow behavior at this location. We have further post-processed the wall shear stress (data not presented here) and found very good correlation with the experimental data. Overall, the simulation results are in very close agreement with the experimental data and were satisfactory, particularly in light of the wide variability of data presented in the challenge.

4. Conclusion

Abaqus/CFD was used to model, simulate and visualize the flow through a benchmark FDA nozzle model and the simulation results were validated by experimental data obtained from the FDA repository and presented in this technology brief. Abaqus/CFD now has the steady state feature, three turbulent models (Spalart-Allmaras model, RNG k-ε and SST k-ω) and a laminar flow model. All of these features were put on test for modeling hemodynamics. The results illustrate the challenging nature of this benchmark and highlight areas where particular user attention is required. This study also revealed that it can be challenging to predict which model type is appropriate for any general medical device geometry for a given flow rate, as laminar, transitional and turbulent flow regions may co-exist in different locations at the same time. This also emphasizes the fact that CFD is not a “push button” technology, and user skill is an important factor in achieving accurate results, while the necessary details in modeling, meshing and analysis set-up play a crucial role in achieving higher levels of accuracy.

5. References

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