Guidelines for Choosing an Appropriate Turbulence Model when Simulating Blood Flows in Cardiovascular Devices

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ABSTRACT

Results are presented from a study to determine which turbulence models are the most appropriate to use in the simulation of cardiovascular flows. The research team undertook a systematic and detailed comparison of the performance of different turbulence models to predict typical velocity fields and shear forces experienced in blood flows. The computational results were validated against experimental data, and guidelines established that will help engineers choose the best models in future studies. The range of turbulence models tested included those specifically developed to predict laminar-to-turbulent transitional flow.

Keywords: computational fluid dynamics, cardiovascular, simulation, turbulence, microfluidics

1 INTRODUCTION

1.1 Computational Fluid Dynamics

Computational Fluid Dynamics (CFD) is a simulation technology that is commonly used in product development and to investigate 'what if…' design scenarios in a controlled, safe, virtual environment. In the last 10 years CFD has helped drive the development of cardiovascular devices which are used to diagnose and treat heart disease and related health problems. The devices are designed to have minimal haemolytic properties and to avoid thrombogenicity and other damage to formed elements in the blood (e.g. von Willebrands monomers). The detrimental effects of high shear stresses on blood have been known for many years. Simulations can be used to measure, assess and compare the performance of different devices across a wide range of operating conditions. Then only the optimal designs need to be fabricated and tested *in vitro*. Although it is generally agreed that simulations are very useful in analysing cardiovascular devices, engineers face significant challenges in generating them.

1.2 Turbulence Modelling Overview

It is quite difficult to define turbulence in either words or mathematically. The flow is so irregular that many researchers have tended to use the word random to describe the fluid motion, and for practical simulation this concept of randomness has prompted the application of statistical tools rather than a deterministic approach to the subject. However, today it is mostly accepted that a turbulent flow has structure and is chaotic rather than random. At any rate it is a phenomenon that is highly complex and stochastic.

It is widely accepted that for incompressible Newtonian fluids, the Navier-Stokes equations coupled with the continuity equation correctly describe the behaviour of flow under laminar and turbulent conditions. However, it is very computationally expensive to calculate all the structures present in a fully turbulent flow. Furthermore, small changes in the initial conditions can lead to large, difficult to predict changes in the long term evolution of the flow variables. So a more practical approach is to predict the overall flow behaviour and mean flow variable quantities. Traditionally there have been four approaches to solving the governing fluid equations. They may either be solved directly - Direct Numerical Simulation (DNS), temporally averaged - Reynolds Averaged Numerical Simulations (RANS), spatially averaged - Large Eddy Simulation (LES) or both spatially and temporally averaged - Detached Eddy Simulation (DES).

Increasing Computational Cost

One-Equation models	• Spalart-Allmaras
Two-Equation models	• Standard K-ε • RNG K-ε • Realizable K-ε • Standard K-ω • BSL K-ω • SST K-ω
Reynolds Stress Model (RSM)	• Linear Pressure-Strain • Quadratic Pressure Strain • Stress-Omega
Transition Models	• K-Kl-ω Transition Model • SST Transition Model
DES	• Spalart-Allmaras • Relizable K-epsilon • SST k-ω
LES	• Scale-Adaptive Simulation
DNS	Directly solving the governing equations

Table 1: The different approaches to turbulence modelling available in the ANSYS CFD (FLUENT) code v.16.0 [1].

Modern commercial CFD packages have a large range of turbulence models available. A detailed description of the models listed in Table 1 can be found in the ANSYS FLUENT Theory Manual [1]. The wide range of competing models developed over more than 40 years of global research and development can often seem daunting. The most common question asked by researchers and industry practitioners alike is therefore ‘which turbulence model is best for my application?’

1.3 Blood flows in Cardiovascular Devices

The rheology of blood makes it a difficult fluid to model. Furthermore, cardiovascular devices may involve complex rotating geometry, the flow fields may have transient features such as moving points of separation and flapping jets, the boundary conditions may be difficult to define and the flow field in the device is likely to contain laminar, turbulent and transitional flow regions.

Despite a considerable amount of research effort being spent on simulating cardiovascular flows [2, 3,], there has been little agreement as to the best approach to modelling the turbulence. As a result there has been a lot of confusion and in recent years authorities such as the U.S. Food Drug Administration (FDA) have called for further investigation and model validation [2]. Furthermore, blind tests on an idealized medical device geometry performed by several experienced CFD groups produced a wide variation in results [2]. This demonstrated that CFD for these applications cannot be considered “push button” technology and emphasised the need for better simulation procedural guidelines.

1.4 Selecting a Turbulence Model

When performing a CFD simulation many assumptions have to be made (modelling goals, geometry, physics, boundary conditions etc.) and there are many potential sources of error (round off, iteration, solution, model, user etc.). It is therefore essential for the CFD Engineer to review the analysis performed and consider the limitations in the context of the modelling goals.

Turbulence modelling can potentially be one of the greatest sources of error in an analysis. Assumptions and simplifications lie at the heart of all the models. The significance of these assumptions should be considered in the context of the flow being analysed.

When selecting a turbulence model a CFD engineer is advised to take several steps:

I. Decide clear modelling goals with a focus on the accuracy required. Furthermore, identify the fluid phenomena that the simulation is seeking to predict.

II. Determine if the flow to be analysed is laminar, turbulent or transitional. Although, in many fluid flows there may be localised areas of laminar and turbulent flows.

III. Review the literature and then select a model that best suites the physics of the problem and the available computational resources.

IV. Validate the selected models for the problem at hand against either experimental data or analytical data when it is available.

V. Perform a sensitivity study on the mesh, turbulence model, wall approach, turbulence model parameters and the turbulent boundary conditions.

VI. Review the limitations of the models and the potential sources of error in the analysis.

The undertaking of these steps should help the CFD engineer reduce the error in the analysis and gain confidence in the results of the simulation performed.

2 SIMULATION RESULTS

2.1 Idealized Medical Device Benchmark

In 2012 Stewart *et al* reported the results from the first computational inter-laboratory study that assessed CFD performance in simulations of an idealized medical device. A group of participants from universities, industry and the U.S. FDA defined the test geometry illustrated in Figure 1. Three independent laboratories generated experimental validation data using particle image velocimetry. This experimental data makes a useful dataset against which CFD simulations can be compared.

The flow rates were chosen to cover all flow regimes – laminar, transition and turbulent [2]. The geometry is orientated so that the flow enters a conical collector, passes through a throat and exits through a sudden expansion.

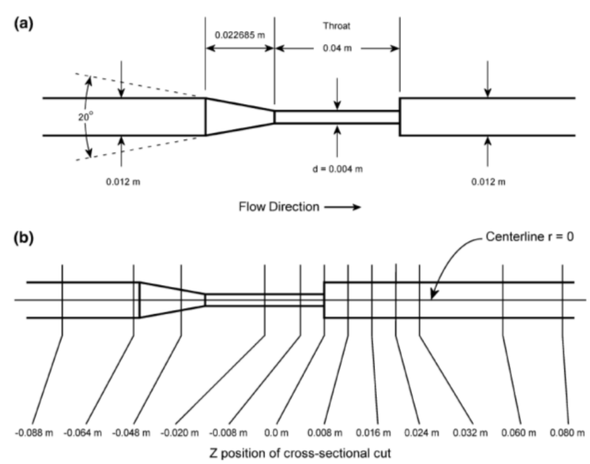

Figure 1: Schematic presentation of the computational domain for the idealized FDA benchmark nozzle geometry [2]

The idealized geometry has many of the characteristics that are found in microfluidic or cardiovascular devices; contractions (streamline curvature, localized acceleration of the flow), expansions (wall separations, recirculating fluid zones, jetting fluid and possibly jet break up) and channel flows (wall shear dominated zones). The present flow has a Reynolds No. of 6,500 based on the throat diameter suggesting that the flow will be mostly turbulent. Consequently the SST k-ω model was employed in the current studies, unless otherwise stated.

2.2 Mesh Sensitivity Study

One of the critical components of any simulation is the sensitivity of the solution to the mesh. The general rule is to have enough mesh to resolve the flow gradients. Various rules and predictive calculations exist to calculate the size of appropriate cells near walls and in free shear layers. However, one good approach is to carry out a grid sensitivity study. Figure 2 illustrates the results of a grid sensitivity study performed on an axisymmetric model of the idealized medical device. The course mesh had 3,350 cells, the medium mesh 11,000 cells and the fine mesh 44,000 cells.

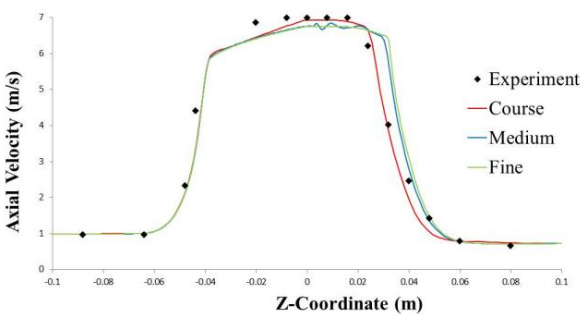

Figure 2: Time averaged axial velocity along the axis line comparing three simulations with different mesh sizes.

2.3 Turbulence Model Comparison

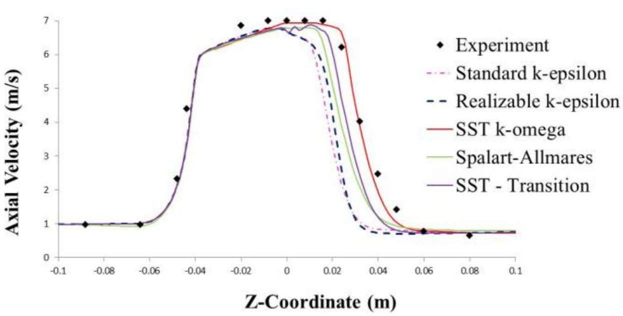

Figure 3: Time averaged axial velocity along the axis line comparing different turbulence models.

Only the SST K-ω model was able to predict the sudden expansion within the confidence levels of the experimental data.

2.4 Comparing Axisymmetric / 3D Results

If the geometry and the flow field are both symmetric around the centerline then an axisymmetric simulation is a valid approach. Axisymmetric simulations significantly reduce the computational effort.

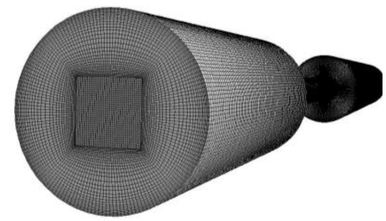

Figure 4: 3D mesh with 1,210,000 cells.

No significant difference was observed between the flow fields calculated using a large 3D simulation and the simpler axisymmetric simulation as illustrated in Figure 4.

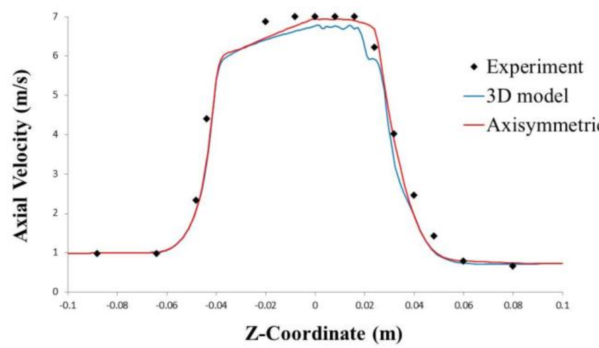

Figure 5: Time averaged axial velocity along the axis line comparing 3D and Axisymmetric models.

2.5 Sensitivity to the Inlet Boundary Conditions

The profile of the boundary condition only affected the flow in the inlet channel and contractor (Figure 6).

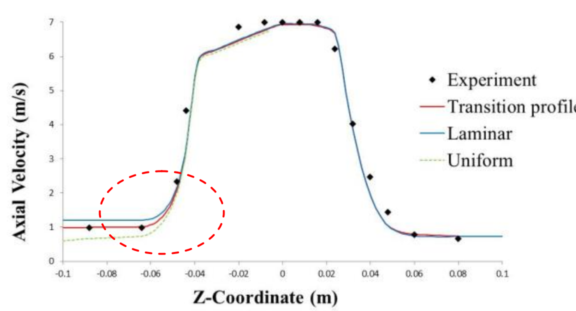

Figure 6: Time averaged axial velocity along the axis line comparing different inlet boundary conditions.

2.6 Transient Features

In some of the simulations which used more refined meshes, vortices were observed forming in the free shear layers after the sudden expansion. These structures appeared to be transient in nature.

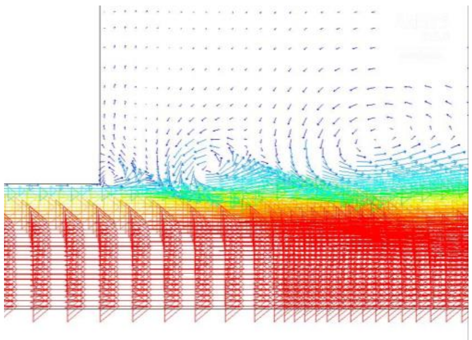

Figure 7: Vortices forming in the free shear layer.

3 SIMULATION CONCLUSIONS

The presented simulations of the idealized medical device benchmark geometry have demonstrated significant sensitivity to the mesh and the turbulence model choice. In addition, the more refined meshes resolved transient structures in the free shear layers, making convergence sometimes difficult to achieve. It is therefore perhaps not that surprising that the blind tests in the original study delivered such a wide range of results.

4 GUIDELINES FOR SELECTING AN APPROPRIATE TURBULENCE MODEL

Considering the modelling complexities associated with blood flows in cardiovascular devices, great care and good practice should be adopted to ensure accurate results. The current paper focuses specifically on guidelines for successfully modelling the effects of turbulence. CFD engineers undertaking a simulation of a cardiovascular flow are advised to:

I. Identify the flow behaviors that need to be captured to correctly predict the shear stresses. Determine if the flow is predominantly turbulent, laminar or transitional. This key information will help inform the CFD engineer which turbulence approach should be adopted.

II. Consider employing a transitional model that may include experimental correlations to trigger the transition onset, when the flow is determined to be in the transitional regime. An alternative approach which is computationally more expensive and less tested is to investigate using DES or LES.

III. Employ a k-ω formulation when the blood flow is determined to be predominantly turbulent. The complex geometry of cardiovascular devices means a turbulence model must be able to predict flow separation from a smooth surface under an adverse pressure gradient, such as in the diffuser section of the idealized geometry modelled, rather than simply from a sharp edge. Models that can integrate to the wall rather than depend on wall functions will therefore likely produce better results. The more sophisticated commercial CFD codes feature models that automatically adapt to the near-wall resolution by blending between wall functions and viscous sublayer models [4]. The present study demonstrated that the SST K-ω models performed the best.

IV. Undertake at least one transient simulation, since it is very likely that the blood flow in cardiovascular devices exhibits transient behavior. The simulation will help determine the source of the transient behavior and determine the effect on the shear stresses in the flow, although static simulations may still yield useful design results.

V. Specify realistic turbulent quantities and profiles at the inflow boundaries. It is reasonable to assume that the overriding flow mechanism in the self-similar region along the walls and areas of separation will be the shear layers. However, the specification of unrealistic boundary conditions such as a uniform velocity will mean the turbulence specified at the inflow boundary will be quickly dissipated and the shear layer development will be delayed [5].

5 FUTURE WORK

Turbulence modelling continues to be one of the driving technologies in CFD [4]. RANS modelling is likely to remain the preferred option for simulating blood flows in cardiovascular and microfluidic devices due to the balance of accuracy and computational resource. However, as computer power continues to grow year on year, the benefits of the DES and LES turbulence approaches will become more attainable. Modelling transitional flows will continue to be a challenge and the topic of continued research.

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