Hybrid RANS-LES Hemolytic Power Law Modeling of the FDA Blood Pump

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Hybrid RANS-LES Hemolytic Power Law Modeling of the FDA Blood Pump

by

Joseph Tarriela

A thesis submitted in partial fulfillment
of the requirements for the degree of
Master of Science in Mechanical Engineering
Department of Mechanical Engineering
College of Engineering
University of South Florida

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Keywords: Hemolysis, Turbulence Modeling, SBES, IDDES, Mechanical Circulatory Support

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Dedication

This work is dedicated to my wonderful girlfriend Maisha Khan for her incredible patience and loving support over the last two years and my family whose encouragement is never ending and faith unwavering.
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Abstract

This study applies the SBES and IDDES hybrid RANS-LES turbulence models along with the K-ω SST model to four flow conditions of the FDA blood pump. Validation of all three turbulence models show good agreement with experimental pressure and velocity fields. Evaluation of turbulent kinetic energy fields for the hybrid models show 80-90+% of kinetic energy is resolved in the rotor and diffuser regions of the pump. Hemolysis power law models were evaluated using the commonly used von Mises stress and additional energy dissipation stress (EDS). Results show viscous and Reynolds stresses computed with the K-ω SST underpredict and severely overpredict the total stress of the hybrid models respectively where EDS shows the best agreement across the three turbulence models. Finally, hemolysis is overpredicted for all turbulence models, though EDS power law results across turbulence models show general agreement in magnitude indicating potential for a universal dissipation based model.
Chapter 1: Introduction

1.1 Heart Failure and Rotary Ventricular Assist Devices

Heart disease is the leading cause of death in America with 696,962 deaths occurring in 2020 according to the CDC [1]. Severe cases of heart disease, such as heart failure rely on either heart transplants or mechanical alternatives such ventricular assist devices (VAD). Due to the increasing number of heart transplant candidates and limited donor supply [2], patients are subject to extended wait times for transplants and risk clinical deterioration and delisting [3]. The use of VADs have been shown to improve survival of heart transplant candidates by reducing the number of patients on transplant lists [3] and as a result, waiting list mortality [4], [5]. Additional therapies utilizing VADS include bridge to recovery as a solution to temporary heart failure where the heart is allowed to recover with mechanical assistance and destination therapy, a terminal solution for patients ineligible for a transplant [3], [4].

The first total artificial heart (TAH) in a human was implanted by Dr. Denton Cooley at the Texas Heart Institute in 1969. Designed with Domingo Liotta, the artificial heart emulated the pulsatile flow of a beating heart with a “pneumatic drive console” [6]. The pneumatic-powered heart was implanted with the intention of acting as a bridge to transplant in a 47-year-old male patient for 64 hours [6]. Although the patient died by complications with the transplanted heart [6], the TAH was a seminal development and demonstrated that humans were able to survive with mechanical circulatory support (MCS) systems [7].

In the decades following, pulsatile pumps maintained the focus within the medical community [8]. In contrast to the prevailing knowledge of the time, Richard Wampler and his
team pioneered implantation of the first rotary pump outputting continuous blood flow to the left ventricle. Known as the Hemopump, the catheter-mounted VAD was intended for use as temporary circulatory support and was first used on a patient in 1988 [9]. The Hemopump was revolutionary for its minimal size, relatively simple design and lack of observed hemolysis despite an axial rotation rate of 27,000 RPM [10]. Although the Hemopump did not achieve commercial success, it is seen as the predecessor of second-generation VADs characterized by axial flow rotary pumps that include the HeartMate II (Abbott Laboratories, Chicago, IL) and Micromed DeBakey (MicroMed Cardiovascular, Inc., Houston, TX). Further advancements led to third generation VADs such as the HeartMate III (Abbott Laboratories, Chicago, IL) and the HeartWare (Medtronic, Minneapolis, MN) where magnetic levitation is used to drive the rotation of a centrifugal impeller [11].

1.2 FDA Round Robin Study

In the development of rotary VADs, one of the primary design considerations is the optimization of fluid flow fields to reduce the magnitude of shear stresses experienced by passing blood. Experimental techniques to visualize flow fields in laboratory settings for VAD evaluation include 2-D particle image velocimetry (PIV) [12] and laser doppler velocimetry [13]. More thorough experimental visualization techniques include 3-D particle tracking velocimetry (3-D PTV) allowing volumetric visualization of experimental flow data as opposed to 2-D techniques [14]. Computational methods such as computational fluid dynamics (CFD) enable researchers and engineers to estimate pump performance and visualize flow fields in three dimensions before a device is physically available to test, drastically reducing lead times for device development.
To better inform design decisions on VADs utilizing CFD in their development, the Food and Drug Administration (FDA) launched the CFD Round Robin Study to evaluate and systematically standardize CFD modeling techniques for blood contacting medical devices [15], [16]. For the study, two idealized medical devices were designed and released freely: a simplified nozzle and centrifugal blood pump, the latter being the focus of this paper [17]. Both models were tested in an interlaboratory effort to acquire flow field and hemolysis data for CFD validation [15], [16], [18], [19].

Since the launch of the study, many researchers provided simulation data on both the nozzle and blood pump. Reynolds Averaged Navier Stokes (RANS), Large Eddy Simulation (LES) and Direct Numerical Simulations (DNS) have been conducted on the nozzle [20]–[22], however, due to the complex nature of the centrifugal pump and computational expense required to sufficiently model the centrifugal pump in LES, a limited number of studies have been published on higher fidelity models of the pump [23]–[25]. This study aims to add to that body of knowledge by utilizing state-of-the-art hybrid RANS-LES models to simulate the centrifugal pump in higher fidelity and test hemolysis modeling techniques against available data.

1.3 Turbulence Modeling

Turbulence flows dominate in the design of VADs and are notorious their difficulty in prediction and correlation to experimental results in engineering flows. Typical modeling approaches for turbulent flows include the RANS and LES models for complex flows. RANS simulations offer the lowest fidelity simulations out of the three model types with the benefit of faster solution times [26]. They solve averaged Navier Stokes equations derived from the decomposition of mean and fluctuating quantities of flow variables [26]. As they solve for the mean components of flow, variations of flow characteristics over time are lost; as such, RANS
simulations are generally suitable for industrial flow applications where a quick general solution is necessary and computational resources are limited [26].

LES simulations, as the name suggests resolve the largest eddies in turbulent flow while modeling the smallest eddies. In terms of turbulent kinetic energy, the largest eddies in a flow reside in lower frequencies of the turbulent kinetic energy spectrum and the smallest eddies occupy the highest frequencies [27]. A low pass filtering operation is applied to the Navier-Stokes equations in order explicitly solve for the largest eddies down to the smallest eddies able to be resolved with respect to the grid and temporal resolution of the simulation. The smallest eddies unresolved in time and space are further modeled by sub-grid scale (SGS) models [26], [27].

Comparatively, LES simulations are much more intensive than RANS simulations due to more stringent grid and temporal requirements. Additionally, wall-bounded LES simulations approach that of DNS in their computational resource requirements [27]. As a workaround to this limitation, hybrid RANS-LES models have been proposed which attempt to use an underlying RANS formulation to model the near-wall boundary layers while switching the LES formulation within the bulk flow regime [28]. This approach has made higher fidelity simulations of industrial problems more approachable and affordable and has been successfully applied to airfoils, turbomachinery and other complex wall bounded flows [28]–[30].

1.4 Hemolysis

Whole blood consists of four primary components: red blood cells (RBC), white blood cells (WBC), platelets and plasma. Red blood cells (RBC) play a key role in the human body’s circulatory system by transporting oxygen and carbon dioxide in and out of the bloodstream. Up
to four oxygen molecules can bind to a single hemoglobin protein within an RBC effectively increasing blood oxygen capacity multiple times over as opposed to oxygen dissolved in blood.

In humans, the hematocrit – or volume percentage of red blood cells to the whole blood ranges from 40-54% in males and 36-48% in females [31]. A drop in hematocrit percentage could signify the occurrence of hemolysis or the breakage of RBCs where the hemoglobin stored internally leaks into the surrounding plasma. Hemolysis can occur as a result of a number of medical conditions including, but not limited to bacterial infection, autoimmune disease and genetic conditions [32], [33].

Hemolysis can also occur as a result of mechanical stresses caused by flow conditions within the blood itself [34]. A RBC possesses a viscoelastic cell membrane which allows the cell to deform under mechanical stress and revert to its original biconcave shape [35]. It has been observed at shear stresses greater than 1 Pa, RBCs take on an ellipsoidal shape. At higher shear stresses, tank-treading occurs where the cell membrane of an RBC begins rotating independent of the internal contents of the RBC [36]. Increasingly higher shear stresses can create pores within the lipid bilayer of the RBC leading to a leakage of hemoglobin [37]. Continued exposure to high stresses can cause the RBC to fully rupture and leak the full contents of the cell into the surrounding plasma.

It has been widely documented that hemolysis occurs as a result of shear stress and exposure time [38]. Several researchers have attempted to quantify the threshold for hemolysis across a range of laminar and turbulent flows, shear stresses, exposure times, experimental setup, and hematocrit. Results from these studies reported many different threshold stresses and exposure times across several different flows [38], [39]. Additionally, the type of stress correlated with hemolysis has been hotly debated. Many authors have correlated mechanical
hemolysis with Reynolds stress, viscous stress, and turbulent dissipation rate among other causes, however a consensus on the mechanism causing mechanical hemolysis is yet to be reached.

1.5 Scope

The intended scope of this thesis is to benchmark the blood pump utilizing URANS modeling with the K-ω Shear Stress Transport (SST) model and two types of hybrid models: the Stress Blended Eddy Simulation (SBES) and the Improved Delayed Detached Eddy Simulation (IDDES). The intent of this study is to benchmark these hybrid models against experimentally PIV data from interlaboratory studies, as well as relative comparisons to more commonly used RANS modeling of the pump. In this study three of the six laboratory tested flow conditions will be evaluated for all models.

In addition to flow modeling, hemolysis power-law models are also evaluated for both RANS and hybrid model cases. As hemolysis has been previously correlated to the shear stresses in fluid flow, this study also aims to evaluate the application of Reynolds stress, viscous stress, and a combination of the two stresses for hemolysis prediction in addition to a scalar stress as a function of turbulent energy dissipation rate.
Chapter 2: Theory and Model Equations

2.1 Turbulence Modeling

2.1.1 Governing Equations

In solving any fluid problem, mass, momentum, and energy must be conserved. For any transfer of mass and energy in and out of a closed system, both quantities must remain constant over time. In a fluid system, the mass conservation can be expressed as the continuity equation:

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0
\]

This can be simplified for incompressible, constant density flows to:

\[
\nabla \cdot \mathbf{u} = 0
\]

Momentums in fluid systems are governed by the Navier-Stokes (N-S) equations. Derived from applying Newton’s second law to continuous fluid motion and considering pressure and viscous forces, the N-S equations can model a variety of natural phenomena and is expressed as:

\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \rho \mathbf{u} \cdot \nabla \mathbf{u} = -\nabla p + \mu \nabla^2 \mathbf{u}
\]

where \( u \) is the velocity, \( p \) is the pressure and \( \mu \) is the dynamic viscosity.

The deformation a particle experiences within a flow can be expressed as the change in velocity with respect to position. Subsequently, the rate of strain tensor can be expressed as

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]
For Newtonian fluids, the deformation of a fluid element is assumed to be proportional to the stress acting on the fluid element. Using viscosity as a proportionality constant, the stress tensor acting on a fluid element can be expressed as

$$\tau_{ij} = 2\mu S_{ij}$$  \hspace{1cm} (2.5)

where $\tau_{ij}$ is the viscous stress tensor, stemming from the usage of the dynamic viscosity $\mu$.

### 2.1.2 Reynolds Averaged Navier Stokes Modeling

#### 2.1.2.1 K-ω SST Model Equations

In this thesis, the primary RANS model used is the K-ω Shear Stress Transport (SST) model introduced by Menter et al. The K-ω SST model is a two-equation turbulence model closed by an eddy-viscosity model. On its own, it is a hybrid model combining the wall-modeling properties of the Wilcox K-ε model and the free stream modeling capabilities of the K-ε models in the bulk flow [40].

The K-ω SST implements a blending function $F_1$ dependent on wall distance multiplied by the final term in Equation 2.7 where the value of $F_1$ determines if the model works in the K-ω or K-ε framework. The model equations for the K-ω SST model are shown as:

$$\frac{\partial \rho k}{\partial t} + \frac{\partial \rho u_j k}{\partial x_j} = P_k - \beta^* \rho\omega k + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_j} \right]$$  \hspace{1cm} (2.6)

$$\frac{\partial \rho \omega}{\partial t} + \frac{\partial \rho u_j \omega}{\partial x_j} = \frac{\gamma}{\nu_e} PV - \beta \rho \omega^2 + \frac{\partial}{\partial x_j} \left[ (\mu + \sigma_\omega \mu_t) \frac{\partial \omega}{\partial x_j} \right] + 2(1 - F_1) \frac{\rho \sigma_\omega^2}{\omega} \frac{\partial k}{\partial x_j} \frac{\partial \omega}{\partial x_j}$$  \hspace{1cm} (2.7)

where Equation 2.6 is known as the turbulent kinetic energy equation (TKE) and Equation 2.7 is known as the specific dissipation rate equation as $k$ is the turbulent kinetic energy and $\omega$ is the specific dissipation rate. The term $P_k$ in the TKE equation is defined as the production of turbulent kinetic energy given as
\[ \bar{p}_k = \min \left[ \mu_t \frac{\partial u_j}{\partial x_j} \left( \frac{\partial u_i}{\partial x_i} + \frac{\partial u_j}{\partial x_j} \right), 10 \cdot \beta^* \rho k \omega \right] \]  

(2.8)

The minimum operator in Equation 2.8 acts as a production limiter to prevent excessive turbulence generation in stagnation regions. The dynamic eddy-viscosity is given as:

\[ \mu_t = \frac{\rho a_1 k}{\max(a_1 \omega, \omega F_2)} \]  

(2.9)

The blending function \( F_1 \) reads as

\[ F_1 = \tanh \{ \text{arg}_1 \} \]  

(2.10)

\[ \text{arg}_1 = \min \left[ \max \left( \frac{2\sqrt{k}}{\beta^* \omega y}, \frac{500\nu}{y^2 \omega} \right), \frac{4\sigma \omega k}{\omega F_2} \right] \]  

(2.11)

where \( F_1 \) is bounded with a maximum and minimum value of 1 and 0 and \( \text{arg}_1 \) is dependent on the distance to the closest wall \( y \). In cells near the wall, \( F_1 \) has a value of 1 in enabling the K-\( \omega \) model. Away from the wall \( F_1 \) has a value of 0 enabling the K-\( \varepsilon \) model. Between the function bounds, \( F_1 \) blends its argument with a hyperbolic tangent function to ensure a smooth transition between the models.

In addition to blending the model equations, \( F_1 \) variables \( \sigma_k, \sigma_\omega, \sigma_{k2}, \) and \( \sigma_{\omega2} \) are empirical constants from the source K-\( \omega \) and K-\( \varepsilon \) equations and are blended by the function \( F_1 \) by the expression

\[ \phi = \phi_1 F_1 + (1 - F_1) \phi_2 \]  

(2.12)

2.1.2.2 Viscous and Reynolds Stress

In solving RANS models of turbulent flow, the N-S governing equations are subject to Reynolds decomposition where instantaneous flow quantities are separated into mean and fluctuating components as seen in Equation 2.13 resulting in the governing RANS equation in Equation 2.14.
Here, \( u \) indicates the instantaneous velocity decomposed into the mean velocity \( \bar{u} \) and instantaneous velocity \( u' \) [27].

\[
\frac{\partial (\rho \bar{u}_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho \bar{u}_i \bar{u}_j) = - \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \rho u'_i u'_j \right] \tag{2.14}
\]

This results in two forms of stress: the first being \( \mu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) \) or the viscous stress tensor and the second term \( -\rho u'_i u'_j \) also known as the Reynolds stress tensor [27]. For viscous stress, the tensor components can be computed with mean flow components. For Reynolds stress, the fluctuating components \( u'_i \) result in the RANS equations becoming an underdetermined system of nonlinear equations due to the computation of mean components.

The Boussinesq approximation introduces the concept of turbulent or eddy viscosity as a form of momentum transfer from turbulent eddies analogous to momentum transfer in gasses as a result of Brownian motion of particles [26], [27]. Applied to the Reynolds stress term, the Boussinesq approximation computes the Reynolds stress as a function of mean flow components allowing for the closure of the RANS equations.

\[
-\rho \bar{u}'_i \bar{u}'_j = \mu_t \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) - \frac{2}{3} \rho k \delta_{ij} \tag{2.15}
\]

where \( \frac{1}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} = 0 \) for incompressible flows and \( k \) is the turbulent kinetic energy. Note the overbar representing the mean velocity component is dropped for simplification in the Equation 2.15.

2.1.2.3 Total Energy Dissipation

From applying Reynolds decomposition to the instantaneous energy equation, the mean kinetic energy equation is expressed as [27]:

\[
u = \bar{u} + u'
\]
\[ \frac{\overline{D(E)}}{Dt} + \nabla \cdot \overline{T} = -\overline{\varepsilon} - \varepsilon' \quad (2.16) \]

\[ \overline{E} = \frac{1}{2} \langle U \rangle \cdot \langle U \rangle \quad (2.17) \]

\[ \overline{T} = \langle U_j \rangle \langle u'_i u'_j \rangle \frac{\partial \langle U_i \rangle}{\partial x_j} + \frac{\langle U_j \rangle \langle p \rangle}{\rho} - 2\nu \langle U_j \rangle \overline{S}_{ij} \quad (2.18) \]

The overall dissipation sink term on the right-hand side of Equation 2.16 split into mean and fluctuating components resulting from the averaging operation, \( \overline{\varepsilon} \) and \( \varepsilon' \) respectively. The two terms then read as

\[ \overline{\varepsilon} = 2\nu \overline{\varepsilon}_{ij} \overline{\varepsilon}_{ij} \quad (2.19) \]

\[ \varepsilon' = -\langle u'_i u'_j \rangle \overline{S}_{ij} \quad (2.20) \]

where \( \overline{S}_{ij} \) is the average strain rate. Given that only the deviatoric part of the Reynolds stress tensor affects dissipation, \( \varepsilon' \) is restated as

\[ \varepsilon' = -\left( \langle u'_i u'_j \rangle - \frac{2}{3} k \delta_{ij} \right) \overline{S}_{ij} \quad (2.21) \]

where \( k \) is the turbulent kinetic energy. The Boussinesq hypothesis can then be applied to restate the fluctuating dissipation in terms of mean variables as

\[ \varepsilon' = 2\nu_t \overline{S}_{ij} \overline{S}_{ij} \quad (2.22) \]

Physically, the mean dissipation represents the thermalization of the mean kinetic energy due to viscosity and the fluctuating component represents the dissipation of energy by turbulent eddies [27]. The mean dissipation is then referred to as the viscous dissipation (\( \varepsilon_{viscous} \)) and the fluctuating dissipation is known as the turbulent dissipation (\( \varepsilon_{turb} \)). The summation of both represents the total instantaneous dissipation of kinetic energy and is expressed as

\[ \varepsilon_{total} = \varepsilon_{turb} + \varepsilon_{viscous} = 2(\nu + \nu_t) \overline{S}_{ij} \overline{S}_{ij} \quad (2.23) \]
2.1.3 Hybrid RANS-LES Modeling

2.1.3.1 Large Eddy Simulation Overview

Unlike RANS models solving for mean flow quantities, LES models resolve instantaneous flow variables comprised of both the mean and fluctuating components. The N-S equations are subjected to a spatial low-pass filtering operation to filter eddies smaller than the filter width [26]. In Ansys Fluent, the cartesian mesh explicitly acts as the filter and must be refined accordingly [41]. The filtering operation on a variable denoted by an overbar is defined as

$$\bar{\phi}(x) = \int_D \phi(x')G(x,x')dx'$$

where D is the domain and G is the filtering function. Given the definition of a filtered variable, any variable $\phi$ can be split as

$$\phi = \bar{\phi} + \phi'$$

The resulting filtered N-S equations are then given as

$$\rho \frac{\partial \bar{u}_i}{\partial t} + \rho \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \mu \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) = -\frac{\partial \bar{p}}{\partial x_i} + 2\mu \frac{\partial \bar{S}_{ij}}{\partial x_j}$$

$$\bar{u}_i \bar{u}_j = \tau_{ij} + \bar{u}_i \bar{u}_j$$

where $\tau_{ij}$ is the Sub-Grid stress (SGS) tensor.

As small dissipative eddies often reside near the wall the filter width must be adjusted to properly resolve larger eddies in the boundary layer region. This results in the grid resolution requirements for wall-bounded LES models increase exponentially [26]. Likewise for temporal resolution, time-step size decreases as mesh refinement increases leading to increasingly small global time-steps as a consequence of near-wall grid refinement. Additionally, complex geometries may increase meshing requirements due to varying levels of curvature across the
domain. As mentioned previously, hybrid models attempt to cover the boundary layer region with an underlying RANS region to reduce both spatial and temporal requirements globally relative to full LES simulations.

2.1.3.2 IDDES Model Equations

2.1.3.2.1 Detached Eddy Simulation

The Improved Delayed Detached Eddy Simulation (IDDES) is a hybrid model of the Detached Eddy Simulation (DES) family initially introduced by Spalart et al. [42]. Originally built on the Spalart-Allmaras (S-A) RANS model, the DES model uses the turbulent length scale computed locally to determine if the grid is small enough to resolve the turbulent eddies and therefore switch to LES. Near the wall, the RANS model utilizes a wall distance, $d$, and a DES filter width defined by Equation 2.28 where $C_{DES}$ is an empirical constant and $\psi$ is a low-Reynolds number correction function. The variable $\Delta_{max}$ represents the maximum local grid spacing ($\max[\Delta_x, \Delta_y, \Delta_z]$).

$$\Delta_{DES} = C_{DES} \psi \Delta_{max}$$ (2.28)

Strelets [43] extended the application of the DES formulation to the $K-\omega$ SST model by modifying the RANS length scale enclosed within the energy dissipation sink term of Equation 2.6 with a DES length scale. The modifications later noted by Menter et al. [44] are as follows:

$$\beta^* \rho k \omega = \frac{\beta^* \rho k^2}{l_{RANS}} = \beta^* \rho \omega F_{DES}$$ (2.29)

$$l_{RANS} = \frac{k^2}{\beta^* \omega}$$ (2.30)

$$F_{DES} = \max\left[\frac{l_{RANS}}{C_{DES}\Delta_{max}}, 1\right]$$ (2.31)
2.1.3.2.2 Delayed Detached Eddy Simulation

The original DES model had issues in the RANS-LES transition region where grid refinement in the boundary layer may be too fine and the DES length scale would cause a premature switch to LES mode. Primarily seen in complex geometries with varying levels of grid-refinement, this switch results in a scenario termed Modeled Stress Depletion (MSD) where and modeled stresses are reduced in this transition. Additionally, the mesh dependency of the model results in early flow separation, termed “Grid-Induced Separation” (GIS) [45].

Spalart et al. [46] proposed an improvement to his original model where he introduced a blending function of the RANS and LES length scale in attached boundary layer flow region such that the new DES length scale reads:

\[ l_{DDES} = l_{RANS} - f_d \max [0, l_{RANS} - \Delta_{DES}] \]  \hspace{1cm} (2.32)

Spalart also incorporated a shielding function to the newly coined Delayed Detached Eddy Simulation (DDES) model so that the boundary layer became strongly dependent on the eddy viscosity of the Spalart-Allmaras model as defined in Equations 2-33 and 2-34 as a preventative measure against GIS.

\[ f_d = 1 - \tanh [(8r_d)^3] \]  \hspace{1cm} (2.33)

\[ r_d = \frac{\mu + \mu_t}{\rho \max[\sqrt{\nu_{i,j}u_{i,j}}]} \]  \hspace{1cm} (2.34)

Gritskevich et al. [47] adapted the DDES and IDDES for use with the K-ω SST model by recalibrating constants used in the \( f_d \) blending function. The recalibrated functions for the SST-IDDES model read as:

\[ f_d = \tanh [(20r_d)^3] \]  \hspace{1cm} (2.35)

\[ r_d = \frac{\mu + \mu_t}{\rho k^2 y^2 \sqrt{\frac{1}{2}(S^2 + \omega^2)}} \]  \hspace{1cm} (2.36)
2.1.3.2.3 Improved Delayed Detached Eddy Simulation Model

The Improved Delayed Detached Eddy Simulation (IDDES) advances the DDES model by including wall-modeled LES (WMLES) functionality [48]. Within the IDDES model, if inflow conditions do not include turbulent content, the IDDES falls back to its DDES capability using the length scale in Equation 2-32. If inflow conditions are unsteady, include turbulent content and the grid is fine enough to resolve the largest eddies in the boundary layer, the WMLES branch is activated. The length scale for this IDDES arm reads as:

\[ l_{WMLES} = f_\beta (1 + f_e) l_{RANS} + (1 - f_\beta) \Delta_{DES} \]  

(2.37)

The empirical blending function \( f_\beta \) scales from 0 to 1 corresponding to LES and RANS modes respectively.

\[ f_\beta = \min\left[2e^{-9\alpha^2}, 1\right] \]  

(2.38)

\[ \alpha = 0.25 - \frac{d}{\Delta_{max}} \]  

(2.39)

The function \( f_e \) offers protection from MSD at the interface of RANS and LES zones and provides a solution to the log-layer mismatch in previous DES models. In the SA-IDDES model, an optional Reynolds number correction is applied, however in the SST-IDDES model, this is disregarded and \( f_e \) reads as:

\[ f_e = \max\left[(f_{e_1} - 1), 0\right] \]  

(2.40)

where

\[ f_{e_1} = \begin{cases} 2 e^{-11.09 \alpha^2} & \alpha \geq 0 \\ 2 e^{-9.0 \alpha^2} & \alpha \leq 0 \end{cases} \]  

(2.41)

\[ f_{e_2} = 1 - \max \left[ \tanh \left( c_l^2 r_d l \right)^{3/2} \right], \tanh \left( c_l^2 r_d l \right)^{10} \right] \]  

(2.42)
The IDDES model also conveniently features a method to switch between the DDES and WMLES modes when resolved turbulent eddies are present in the boundary layer by combining previously defined blending functions into a singular length scale.

\[ l_{IDDES} = \tilde{f}_d (1 + f_\omega) l_{RANS} + (1 - \tilde{f}_d) l_{LES} \]  \hspace{1cm} (2.43)

where

\[ \tilde{f}_d = \max[1 - f_{d_t}, f_\beta] \]  \hspace{1cm} (2.44)
\[ f_{d_t} = 1 - \tanh \left( \left( 8 r_{d_t} \right)^3 \right) \]  \hspace{1cm} (2.45)
\[ l_{LES} = \min \{ C_w \max[d, \Delta_{max}], \Delta_{max} \} \cdot (C_{DES1} \cdot F_1 + C_{DES2} \cdot (1 - F_1)) \]  \hspace{1cm} (2.46)

The quantity \( C_w \) is a parameter obtained by calibration from channel flow simulations, \( \Delta_{max} \) is the maximum edge length of a cell; the values of \( C_{DES1}, C_{DES1} \) and formulations for \( F_1 \) and \( F_2 \) can be found in the work of Gritskevich et al. [47]. Amending this model into a two-equation form, the dissipation term can be formulated similar to the DES and DDES models as:

\[ \rho \varepsilon_{IDDES} = \rho \beta^* k \omega \frac{l_{RANS}}{l_{IDDES}} = \rho \beta^* k \omega F_{IDDES} \]  \hspace{1cm} (2.47)

The associated RANS model for the IDDES model in this work is the two-equation K-\( \omega \) SST model posed by Gritskevich et al. [47]. As such, the appropriate name for the model is SST-IDDES, however from hereon it will be referred to simply as IDDES.

2.1.3.3 SBES Model Equations

2.1.3.3.1 Shielded Detached Eddy Simulation

Another hybrid model analyzed in this thesis is the Stress Blended Eddy Simulation (SBES) model which is built upon the Shielded Detached Eddy Simulation (SDES) model. The SDES model is another variant of the DDES model and improves on the DDES formulation for
two-equation models [49]. The $k$-equation sink term is modified with a blending function based on the DDES blending function:

$$\rho \varepsilon_{SDES} = -\beta^* \rho k \omega F_{SDES}$$ (2.48)

where

$$F_{SDES} = \left[ \max \left( \frac{L_t}{C_{SDES} \Delta_{SDES}} (1 - f_s), 1 \right) - 1 \right]$$ (2.49)

$$\Delta_{SDES} = \max \left[ \sqrt[3]{\nu t}, 0.2 \Delta_{max} \right]$$ (2.50)

The blending function $f_s$ provides improved shielding in the boundary layer and the grid dependency on $\Delta_{SDES}$ provides a more aggressive length scale definition than the DES and DDES models to resolve turbulent scales faster.

2.1.3.3.2 Stress Blended Eddy Simulation

Introduced by Menter et al. [49], the SBES model offers modularity between different RANS and LES formulations allowing users to utilize their validated solvers and models of choice. In addition to the modularity of solvers, the SBES model also more clearly demarcates RANS and LES regions as opposed to the DES family of models as well. The model also includes WMLES capability when in LES mode in regions of sufficient mesh resolution.

Building on the blending properties of the SDES model, RANS and LES components are blended together using an additional blending function $f_{SBES}$.

$$\tau_{ij} = \tau_{ij}^{RANS} f_{SBES} + \tau_{ij}^{LES} (1 - f_{SBES})$$ (2.51)

It can be seen that the model operates in RANS when $f_{SBES} = 1$ and LES when $f_{SBES} = 0$. Additionally, if both the RANS and LES models are eddy-viscosity models, the eddy-viscosity $\nu_t$ can be blended in a similar manner:

$$\nu_t = \nu_t^{RANS} f_{SBES} + \nu_t^{LES} (1 - f_{SBES})$$ (2.52)
2.1.3.4 Sub Grid Stress

Just as RANS models require closure of their corresponding governing equations, LES and hybrid models require the same. From Equation 2.53, the SGS tensor $\tau_{ij}$ is not in terms of filtered velocity components. This gives rise to a similar closure problem as the RANS governing equations when substituted into the filtered N-S equations resulting in:

$$\rho \frac{\partial \bar{u}_i}{\partial t} + \rho \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + 2\mu \frac{\partial \bar{S}_{ij}}{\partial x_j} - \frac{\partial \tau_{ij}}{\partial x_j}$$

(2.53)

One approach to closing the filtered equations is eddy viscosity models, a class of SGS models identical in principle to the RANS approach in employing the Boussinesq hypothesis [26]. For SGS, stresses are computed by

$$\tau_{ij} - \frac{1}{3} \tau_{kk} \delta_{ij} = -2\mu_t \bar{S}_{ij}$$

(2.54)

where $\mu_t$ is the turbulent viscosity, $\tau_{kk}$ is the hydrostatic stress added to the filtered pressure and $\bar{S}_{ij}$ is the resolved strain rate tensor. The SGS model used with the SBES model to compute the turbulent viscosity is the Wall-Adapting Local Eddy Viscosity (WALE) proposed by Nicoud and Ducros [50] model which computes $\mu_t$ as

$$\mu_t = \rho \Delta_s^2 \frac{(S_{ij}^d S_{ij}^d)^{\frac{3}{2}}}{(\bar{S}_{ij} \bar{S}_{ij})^{\frac{5}{2}} (S_{ij}^d S_{ij}^d)^{\frac{5}{4}}}$$

(2.55)

$$\Delta_s = 0.325 \bar{V}^{\frac{1}{3}}$$

(2.54)

$$S_{ij}^d = \frac{1}{2} (\bar{g}_{ij}^2 + \bar{g}_{ij}^2) - \frac{1}{3} \delta_{ij} \bar{g}_{kk}^2$$

(2.55)

$$\bar{g}_{ij} = \frac{\partial \bar{u}_i}{\partial j}$$

(2.56)

$$\bar{g}_{ij}^2 = \bar{g}_{ik} \bar{g}_{kj}$$

(2.57)
The WALE model accounts for the local strain and rotational rates ideally detecting all turbulence structures relevant for kinetic energy dissipation. Additionally, the computed turbulent viscosity of the model tends to zero in pure shear and near walls allowing for improved transitional flow predictions relative to the Smagorinsky SGS model.

For the IDDES model, SGS viscosity is modeled as a function of turbulent kinetic energy and specific dissipation \([47]\) similar to the K-\(\omega\)-SST model as:

\[
\mu_t = \frac{\rho a_1 k}{\max(a_1 \omega, \omega F_2)}
\]

\(F_2 = \tanh(\text{arg}_2^2)\)  \(\quad (2.58)\)

\[
\text{arg}_2^2 = \max \left( \frac{2\sqrt{k}}{C_{\mu} \omega d_w} \frac{500\nu}{d_w \omega} \right)
\]

\(\quad (2.59)\)

\(\quad (2.60)\)

### 2.1.3.5 Total Energy Dissipation

Like the stress tensor, turbulent dissipation in LES and hybrid models is also explicitly evaluated at the largest scales and modeled at the smallest scales according to the filter width \([27]\). Viscous dissipation at resolved scales can be computed with the filtered rate of strain magnitude and viscosity as:

\[
\varepsilon_{\text{resolved}} = \nu |\tilde{S}|^2
\]

where the rate of strain magnitude is defined as:

\[
|\tilde{S}| = \sqrt{2S_{ij} \tilde{S}_{ij}}
\]

\(\quad (2.61)\)

\(\quad (2.62)\)

The SGS contribution of the dissipation rate can then be similarly evaluated as:

\[
\varepsilon_{\text{SGS}} = \nu_t |\tilde{S}|^2
\]

\(\quad (2.63)\)

Then the total instantaneous dissipation for LES would be:

\[
\varepsilon_{\text{LES}} = (\nu + \nu_t) |\tilde{S}|^2
\]

\(\quad (2.64)\)
This expression for the SGS dissipation assumes local equilibrium between production and dissipation of energy where energy from larger scales into a local cell is instantly dissipated in the subgrid portion of said cell. This simplifying assumption means that SGS dissipation can be viewed as the average dissipation energy at the smallest unresolved scales in a cell [27].

As the instantaneous dissipation is computed similarly for hybrid and RANS models, Equation 2.64 can be restated as:

$$\epsilon_{hybrid} = (\nu + \nu_t)|\bar{S}|^2 \quad (2.65)$$

where the rate of strain magnitude and turbulent viscosity is dependent on the local cell position and governing model type.

In a bulk flow LES region, turbulent viscosity generation is a function of the SGS model and the rate of strain magnitude is a function of the filtered velocity field. In RANS regions, turbulent viscosity is likewise computed by the RANS model and the rate of strain magnitude is a function of the mean velocity field.

### 2.2 Computation of Hemolysis

The computation and prediction of hemolysis with CFD typically is approached in two ways. The first, a Lagrangian method, entails releasing a finite number of particles at the inlet of the domain and recording the damage the particle experiences as it travels through the domain at each time step. Each particle path line is tracked through the domain and the cumulative hemolysis computed for each path line is computed with the velocity-weighted average at the outlet [51]. This approach can be computationally affordable depending on the number of finite particles and path lines to be tracked, however, it can be time consuming to postprocess. The primary advantage of the Lagrangian method is that shear stress and hemolytic damage can be computed on the path line accounting for the time-history of an RBC flowing through the
domain. The downside is that a sufficient number of path lines for a complex geometry must be considered and computed as regions of high stress and blood damage may potentially missed if the domain is not sufficiently seeded.

The Eularian approach, which this work focuses on, consists of implementing a linearized power-law model for hemolysis as a source term into a transport equation. The transport equation then solves for the generation and convection of plasma-free hemoglobin \((pfHb)\) in the fluid domain which is computed by the mass weighted average of \(pfHb\) at the flow outlet [52]. The power-law model, introduced by Giersiepen et al. [53] takes the form of Equation 2.66 where the ratio of \(pfHb\) in units \(\frac{mg}{aL}\) to the total concentration of hemoglobin \((Hb)\) is defined in percentage as a function of a scalar shear stress \(\tau\) and exposure time \(t\).

\[
HI\% = (1 - Hct) \frac{pfHb}{Hb} \times 100 = C\tau^\alpha t^\beta
\]  

(2.66)

The Eularian model approach eliminates the need to track path lines as \(pfHb\) is modeled as a scalar convicted through the domain. As the scalar is solved over the entire flow field, the Eularian can identify regions of potential hemolysis generation, however, the time-history of RBC damage is not accounted for.

Hemolysis experiments for the FDA blood pump utilized porcine blood with an adjusted hematocrit of 36 ± 1%, viscosity of 0.0034 \(Pa \cdot s\) and a density of 1030 ± 10 \(\frac{kg}{m^3}\) as reported by Malinauskas et al. [19]. Experimental runtime for the pump was 120 minutes where 1 \(mL\) of blood was drawn every 40 min. Hemolysis found to increase linearly over time throughout the experimental runtime of 120 minutes [19]. Experimental hemolysis results were similarly converted to HI% to compare with CFD results.
It should be stated that the power law model for CFD computations in Equation 2.66 represents the rise in \( pfHb \) for a single flow through of the pump. Or in other words, it represents the hemolysis increase after the computational pump has passed a volume of liquid equivalent to the experimental flow circuit volume. Experimentally, hemolysis collection occurs over several passes through the pump and must be scaled appropriately for comparison. Experimental \( pfHb \) values can be scaled as

\[
pfHb = pfHb_{\text{exp}} \frac{V}{QT} \tag{2.67}
\]

where \( V \) is the volume of the experimental flow loop, \( Q \) is the flow rate, \( T \) is the length of time blood has recirculated through the flow loop and \( Hct \) is the hematocrit in percent. The scaling factor \( \frac{V}{QT} \) adjusts experimental \( pfHb \) values to the rise of a single flow through applied to the HI expression in Equation 2.66. Additionally, in the regression of hemolysis data for power-law model coefficient fitting, hematocrit is accounted for, hence the normalization by \( (1 - Hct) \) in Equation 2.66 [55]–[57].

2.2.1 Eulerian Hemolysis Modeling Approach

In order to implement the power-law model into a CFD solver, an Eulerian technique developed by Garon and Farinas is used [52]. Equation 2.66 is first linearized with respect to time as shown in Equation 2.68:

\[
HI^{1/\beta} = C^{1/\beta} t^{\alpha/\beta} 
\tag{2.68}
\]

A new variable \( H' \) is defined, equivalent to \( HI^{1/\beta} \) and the time derivative is taken.

\[
\frac{dH'}{dt} = C^{1/\beta} t^{\alpha/\beta} \tag{2.69}
\]

Equation 2.69 is then applied to standard transport equation as a source term. Density is multiplied by the source term to preserve dimensionality [41].
\[
\frac{\partial}{\partial t} (\rho H') + \frac{\partial}{\partial x_i} \rho u_i H' = \rho C \frac{1}{\beta} \tau^{\alpha} \]

(2.70)

The scalar transport equation is then implemented in Ansys Fluent as a UDF and solved over a frozen, steady state flow field to initialize the simulation. For transient calculations, flow equations are reenabled and solved in tandem with the scalar transport equations [41].

Table 2.1: Power law model coefficients and shear stress ranges.

<table>
<thead>
<tr>
<th>Model Abbv.</th>
<th>Researchers</th>
<th>Species</th>
<th>( C )</th>
<th>( \alpha )</th>
<th>( \beta )</th>
<th>Shear Stress Range (Pa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>GW</td>
<td>Giersiepen et al.</td>
<td>Human</td>
<td>( 3.620 \times 10^{-5} )</td>
<td>2.416</td>
<td>0.7850</td>
<td>( \tau &lt; 255 )</td>
</tr>
<tr>
<td>HO</td>
<td>Heuser &amp; Opitz</td>
<td>Porcine</td>
<td>( 1.800 \times 10^{-4} )</td>
<td>1.991</td>
<td>0.7650</td>
<td>( \tau &lt; 700 )</td>
</tr>
<tr>
<td>DP</td>
<td>Ding et al.</td>
<td>Porcine</td>
<td>( 6.701 \times 10^{-4} )</td>
<td>1.0981</td>
<td>0.2778</td>
<td>( 25 &lt; \tau &lt; 320 )</td>
</tr>
<tr>
<td>TZ</td>
<td>Zhang et al.</td>
<td>Ovine</td>
<td>( 1.228 \times 10^{-5} )</td>
<td>1.9918</td>
<td>0.6606</td>
<td>( 50 &lt; \tau &lt; 320 )</td>
</tr>
</tbody>
</table>

Commonly used coefficients for the power law model have been experimentally regressed from laminar shear experiments with Couette viscometers. From viscometrical experiments on platelet and RBC damage conducted by Wurzinger et al. [58], [59], Giersiepen et al. developed the power-law correlation and tested the model against in-vitro data on heart valves [53]. Heuser and Opitz [57] published hemolysis data from laminar shear flow experiments on porcine blood conducted with a Couette viscometer in 1980 and the data was later fitted to the power law model by Song et al. [60]. Similarly, Ding et al. and Zhang et al. conducted shear experiments on various blood species using specially adapted Couette viscometers and different blood species [55], [56]. The coefficients for Equation 2.66 used in this study are shown in Table 2.1.
2.2.2 Hemolytic Stresses in Turbulent Flow

The type of stress used to correlate and estimate hemolysis in turbulent flows has been thoroughly debated. Hemolysis in turbulent flows have previously been seen to exponentially increase relative to increasing Reynolds number by Kameneva et al. [39], though the mechanical mechanism for hemolysis is still unknown. In an attempt to determine an incipient hemolysis threshold, Sallam and Hwang [61] experimentally observed the flow field of a turbulent jet with laser doppler anemometry and determined that a Reynolds Stress of $400 \text{ Pa}$ at an exposure time of $10E^{-5} \text{s}$ induced hemolysis. Similar studies by Grigioni et al. [62] and Lu et al. [63] correlated incipient hemolysis with Reynolds stress thresholds of 600 and 800 Pa respectively.

Alternatively, turbulent energy dissipation has been proposed as a better correlation for hemolysis. Bluestein and Mockros [64] were among the first to establish a power relationship between energy dissipation and hemolysis. Jones [65] argued that Reynolds stresses are derived from Reynolds decomposition of the N-S equations and were not true stresses on RBCs and proposed that instantaneous viscous stress on the scale of red blood cells should be investigated. He showed that a turbulent viscous shear stress acting as a hemolytic force should be proportional to the square root of the viscous dissipation of turbulent energy. Kameneva et al. [39] later postulated that turbulent hemolysis may occur due to Kolmogorov scale eddies acting on RBCs. As turbulent energy dissipation occurs at the smallest scales of the turbulent energy cascade [27] and TVSS is a scalar measure of stress as a result of small scale velocity gradients in terms of dissipation, TVSS can be seen as the scalar viscous stress energy dissipating eddies at the Kolmogorov scale. This led to Yen et al. [66] to characterize the hemolytic threshold of TVSS by measuring the flow field of a submerged axisymmetric jet finding a Reynolds stress threshold of 517 Pa and a TVSS threshold of an order of magnitude less.
2.2.3 Scalar Shear Stress for the Hemolysis Power Law Model

The correct form of the scalar shear stress has been a source for debate among researchers where different definitions have been applied to the power-law model. The variations stem from disagreement in the approach of quantifying the stress tensor into a single scalar value for three-dimensional shear flows. To evaluate the differences between stresses in RANS calculations, both the Reynolds and viscous stress tensors and scalar stresses are individually computed. By matrix addition the Reynolds and viscous stress tensors in Equation 2.15 and Equation 2.5 respectively are summed and the total stress tensor is computed as

\[ \tau_{\text{total}} = \tau_{\text{viscous}} + \tau_{\text{Reynolds}} \]  

(2.71)

Commonly, the Von Mises stress criterion, or maximum distortion criterion is applied when computing a scalar shear stress. Von Mises stress criterion is based on the distortion energy associated with shape change of a material. In solid mechanics, it represents the point where a solid begins to yield [67]. In the context of hemolysis, it represents the combination of normal and shear stresses acting on a point within the computational domain where hemolysis may occur.

Mathematically, the Von Mises criterion can be expressed as the second invariant of the deviatoric stress tensor:

\[ \tau_{VM} = \sqrt{3J_2} \]  

(2.72)

Substituting for stress tensor components, the von Mises stress is expressed as:

\[ \tau_{VM} = \left( \frac{1}{2} \left[ (\tau_{11} - \tau_{22})^2 + (\tau_{22} - \tau_{33})^2 + (\tau_{33} - \tau_{11})^2 + 6(\tau_{12}^2 + \tau_{13}^2 + \tau_{23}^2) \right] \right)^{\frac{1}{2}} \]  

(2.73)

This form of the scalar shear stress has been applied by several researchers including Taskin et al. [51], Fraser et al. [68], as well as Garon and Farinas [52] in their original transformation of the power-law model into a scalar transport equation. Faghih et al. [69]
demonstrated that an appropriate scalar stress (modified Von Mises stress) should reduce to the shear stress for a simple shear flow where $\sigma_{12} = \sigma_{21} = \tau$ and provided a simple change for the constant where

$$\tau_{VM}^{mod} = \frac{1}{\sqrt{3}} \tau_{VM}$$

(2.74)

The $\tau_{VM}^{mod}$ is used hereonafter to represent the von Mises scalar shear stress in hemolysis computations.

Per Jones [65], the TVSS should be proportional to the square root of the dissipation of turbulent energy. As turbulent dissipation occurs across the entire range of the Kolmogorov microscales both modeled and resolved, Wu et al. [76] expressed the TVSS in terms of the total energy dissipation in a turbulent flow termed energy dissipation stress (EDS).

$$\tau_{EDS} = \sqrt{\epsilon^{Total} \mu \rho}$$

(2.75)

where $\epsilon^{Total}$ is the summation of turbulent and viscous energy dissipation in RANS models and the summation of the resolved and SGS dissipation of the hybrid models from Eq. 2.23. Similar to Reynolds stress, EDS is not a true stress, but rather represents the stress imparted by small energy dissipating eddies applied to a red blood cell at the Kolmogorov microscale level. Regardless of flow regime, dissipation occurs in all viscous flows and this scalar stress allows for an expression equivalent across flow regimes and turbulence models.
Chapter 3: Methods

3.1 Flow Conditions

In this study, four of the six flow conditions published by the FDA were simulated and analyzed. As seen in Table 1, Conditions 1, 4, 5 and 6 were selected. The fluid was assumed to have a constant density of \( \frac{1035 \text{ kg}}{\text{m}^3} \). Although blood is widely known to be a non-Newtonian fluid with exponentially decreasing viscosity associated with increasing shear rates, a constant viscosity of \( 0.0035 \text{ Pa} \cdot \text{s} \) due to the continuously high shear rates within a centrifugal pump.

Table 3.1: Flow conditions evaluated for the FDA blood pump.

<table>
<thead>
<tr>
<th>Flow Condition</th>
<th>Inlet Flow Rate ( \frac{L}{s} )</th>
<th>Pump Speed ( \text{RPM} )</th>
<th>Inlet Turbulent Intensity</th>
<th>Pump Reynolds Number</th>
<th>Average Inlet Velocity ( \frac{m}{s} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.5 ( \frac{L}{s} )</td>
<td>2500 RPM</td>
<td>4%</td>
<td>209338</td>
<td>0.37 ( \frac{m}{s} )</td>
</tr>
<tr>
<td>4</td>
<td>6.0 ( \frac{L}{s} )</td>
<td>2500 RPM</td>
<td>7%</td>
<td>209338</td>
<td>0.88 ( \frac{m}{s} )</td>
</tr>
<tr>
<td>5</td>
<td>6.0 ( \frac{L}{s} )</td>
<td>3500 RPM</td>
<td>7%</td>
<td>293073</td>
<td>0.88 ( \frac{m}{s} )</td>
</tr>
<tr>
<td>6</td>
<td>7.0 ( \frac{L}{s} )</td>
<td>3500 RPM</td>
<td>7%</td>
<td>293073</td>
<td>1.03 ( \frac{m}{s} )</td>
</tr>
</tbody>
</table>

3.2 Geometry

The blood pump, seen in Figure 3.1, was obtained from the NCI database containing computer aided design (CAD) files and velocity validation data for FDA Round Robin study [17]. It generalizes the important components of blood pumps including simplified rotor
impellers, volute, and cutwater region. The inlet and outlet piping have a diameter of 12 mm leading to and from the rotor housing. The rotor itself has a diameter of 0.052 m, a thickness of 0.004 m and four impellers that sit at 90° angles at a height of 0.003 m tall. The experimental models were manufactured with acrylic with an estimated wall roughness of $Ra < 0.6 \, \mu m$ [19].

![Diagram of a computational pump domain](image)

**Figure 3.1:** A: Computational pump domain. B: Illustrates the location of the mid-blade plane through the rotor and outlet pipe volumes. C: Sampling locations along mid-blade plane indicated by red lines. Q1 refers to sampling line through quadrant 1 of the rotor. Q2 refers to sampling line through quadrant 2 of the rotor. D1-D4 indicate diffuser slices by distance ($x = 0.02 \, m, 0.025 \, m, 0.03 \, m, 0.035m$) to the origin at the center of the rotor hub shown by a red dot.

The CAD model was partitioned to create two fluid domains resulting in a non-conformal mesh interface separating them. One region consisted of the rotor and surrounding fluid, the other consists of the rest of the model. The interface boundaries were defined as the midpoint distance between the solid rotor domain and its nearest parallel wall. This partitioning allows for the use of the sliding mesh technique where a rotating domain can slide against a static domain.
Information from nodes along the interface are interpolated to the neighboring cells across the interface allowing for the explicit modeling of rotor movement in the model for transient simulations. For steady state simulations, the Moving Reference Frame (MRF) is utilized where dynamic movement of a partition is modeled within the momentum equations and the entirety of the mesh remains static [41].

3.3 Meshing

Meshes were generated in Ansys Fluent Meshing with a poly-hexacore volume mesh. Each mesh was generated with a body of influence enveloping the rotor and a portion of the outlet pipe. For the 15, 19 and 24 million cell meshes, a face of influence was used to refine the fillet where the outlet pipe meets the rotor housing in order to preserve the curvature of the local geometry. In all cases, the inlet piping was coarsened relative to the rest of the geometry as this region was intended to be modeled in RANS as this portion of the geometry was not of significant interest to the rest of the study.

Figure 3.2: Mesh illustrations of 19M Hybrid models. A displays volume mesh on slices through domain. B displays surface mesh of rotor domain. C displays surface mesh at the fillet interface between the outlet pipe and rotor housing.
Steady state simulations were conducted for each mesh utilizing the MRF technique and K-ω SST model to conduct a mesh independence study. Five meshes were tested and pressure head rise was monitored over the pump. The relative error to the experimental mean pressure rise was used as the comparison metric. For transient RANS cases, the 12 million cell mesh was utilized and for the hybrid models, the 19 million cell mesh was used.

Figure 3.3: Solution dependance of pressure head in mmHg to cell count.

Table 3.2: Mesh convergence study information.

<table>
<thead>
<tr>
<th>Mesh Elements (million)</th>
<th>Boundary Layers</th>
<th>Growth Rate</th>
<th>Mean Rotor $y^+$</th>
<th>Pressure Head (mmHg)</th>
<th>Relative Error to Finest Mesh</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.4</td>
<td>5</td>
<td>1.2</td>
<td>1.081</td>
<td>187.22</td>
<td>15.24%</td>
</tr>
<tr>
<td>8.15</td>
<td>7</td>
<td>1.2</td>
<td>0.975</td>
<td>149.01</td>
<td>8.28%</td>
</tr>
<tr>
<td>12</td>
<td>10</td>
<td>1.2</td>
<td>0.387</td>
<td>167.83</td>
<td>3.31%</td>
</tr>
<tr>
<td>15</td>
<td>10</td>
<td>1.2</td>
<td>0.355</td>
<td>161.4</td>
<td>0.65%</td>
</tr>
<tr>
<td>19</td>
<td>10</td>
<td>1.2</td>
<td>0.302</td>
<td>162.46</td>
<td>-</td>
</tr>
</tbody>
</table>
3.4 Spatial Resolution for LES

Following the mesh independence study, the suitability of the mesh for LES simulations was evaluated as the mesh resolution directly correlates to how much turbulent kinetic energy is explicitly resolved in the simulation. A single-grid estimator to evaluate potential meshes for production use was adopted [70]. From an initial RANS simulation conducted on the mesh of interest, the integral length scale $l_0$ can be computed from the turbulent kinetic energy $k$ and specific dissipation rate $\omega$.

$$l_0 = \frac{\sqrt{k}}{C_\mu \omega}$$
$$C_\mu = 0.09$$

To determine the resolution of the mesh, the ratio of the integral length scale to the local cell length $\Delta$ is taken and qualitatively examined through contours of the domain. For at least 80% of the turbulent kinetic energy in the mesh to be explicitly resolved, a ratio value of 5 is required. For 90%, a ratio of approximately 13 is required.

For each case, a steady state simulation was conducted with the K-\(\omega\) SST model and MRF technique. These simulations were then evaluated with contours of $\frac{l_0}{\Delta}$ to ensure the appropriate areas of the mesh were resolved for LES. As seen in Figure 3.4, the contours show that near-wall regions are under-resolved for LES as intended. Using hybrid models, these areas will be evaluated with the underlying RANS formulation. The inter-rotor regions appear to be very well resolved in addition to the blade gap from the outer edge of the rotor to the rotor housing. Additionally, the outlet diffuser is well resolved in the 80% range of the $\frac{l_0}{\Delta}$ ratio indicating that the mesh used is suitable for use in LES cases. Due to differences in RANS and
LES formulations, this qualitative analysis is not particularly robust, however is a good indicator of potential results and useful in the initial refinement of an LES mesh.

Figure 3.4: Estimated resolved turbulent kinetic energy in the 19M cell mesh for condition 1.

3.5 Temporal Resolution for LES

The Courant–Friedrichs–Lewy (CFL) condition was used as the criterion for determining the time-step size of the model and is expressed in terms of the Courant number, time-step $\Delta t$, local cell length $\Delta$ and local velocity magnitude $U$ [27].

$$C = U \frac{\Delta t}{\Delta} \quad (3.2)$$

The Courant number in Equation 3.2 acts as a general indicator of how fast information travels across computational grid cells when solving discretized partial differential equations. For a Courant number less than 1, information resides within a given cell for at least a single time-step. Courant values greater than 1 indicate that information can skip cells in a given timestep. When the Courant number exceeds the value of 1, numerical instabilities may propagate throughout the solution domain and cause divergence of the solution. Using the same steady
state solutions as the turbulent kinetic energy analysis. Equation 3.2 was reorganized to solve for the time-step as shown in equation 3.3 for a Courant number of 1.

\[ \Delta t = \frac{\Delta}{U} \] (3.3)

To determine the required timestep for a cell given a Courant number of 1, Equation 3.3 was evaluated and visualized in Figure 3.5. From Figure 3.5, the largest timesteps for a Courant number of 1 are seen in the inlet and outlet pipes. Additionally, the smallest timesteps are seen in the impeller wake where small eddies are seen. Although small time steps are required for wall-bounded LES flows, the near wall time step requirement is relaxed as the walls for hybrid models are computed by the underlying RANS model. A summary of timesteps chosen can be found in Table 3.3.

![Figure 3.5: Contour slices through pump colored by time step required for a local Courant number of 1.](image-url)
Table 3.3: Time step values for RANS and hybrid models at 2500 and 3500 RPM

<table>
<thead>
<tr>
<th>Turbulence Model</th>
<th>Impeller Rotation Speed (RPM)</th>
<th>Timestep (sec)</th>
<th>Angular Degrees Traveled</th>
</tr>
</thead>
<tbody>
<tr>
<td>RANS</td>
<td>2500</td>
<td>1/15,000</td>
<td>1°</td>
</tr>
<tr>
<td></td>
<td>3500</td>
<td>1/21,000</td>
<td>1°</td>
</tr>
<tr>
<td>Hybrid</td>
<td>2500</td>
<td>3/200,000</td>
<td>0.225°</td>
</tr>
<tr>
<td></td>
<td>3500</td>
<td>3/280,000</td>
<td>0.225°</td>
</tr>
</tbody>
</table>

3.6 Boundary Conditions

PIV data captured and averaged from experiments performed on the pump inlet allowed for the approximation of inlet velocity profiles upstream of the pump. A 5th order polynomial was regressed to the experimental profiles. The resulting functions were input into Ansys Fluent as a named expression and applied as an inlet boundary condition. The inlet profiles were validated by initializing the simulation and cross-checking the volumetric flowrate generated by the initialized solution. The 2.5 $\frac{L}{min}$, 6 $\frac{L}{min}$, and 7 $\frac{L}{min}$ profiles matched experimental flowrate values within 0.5%. At the outlet, a zero-pressure condition was applied where pressure change was monitored at the inlet.

For the computation of hemolysis, scalar source terms were expressed as User Defined Scalars within a User Defined Function (UDF) in Ansys Fluent [71]. The code explicitly calculates modified Von Mises and EDS stresses by looping through each cell at every iteration and computes each scalar transport equation. Physically, the computation of the scalar equations represents the generation of hemolysis within a computational cell and its resultant convection to the outlet of the domain. Boundary conditions for all scalar equations then include a value of
zero at the inlet and a flux of zero at all walls and the domain outlet to reflect this. A sample of the code can be found in Appendix A.

![Experimental velocity profiles at domain inlet overlaid with regressed profiles for CFD for three flow rate conditions.](image)

**Figure 3.6:** Experimental velocity profiles at domain inlet overlaid with regressed profiles for CFD for three flow rate conditions.

### 3.7 Numerical Methods

For transient K-ω SST models, the SIMPLE spatial discretization scheme was used along with 2\(^{nd}\) order schemes for pressure and 2\(^{nd}\) order upwind schemes for momentum, turbulent kinetic energy, and specific dissipation rate. For both the SBES and IDDES models, the SIMPLC spatial discretization scheme was used with bounded central differencing for the momentum equations. All scalar transport equations were solved with a 2\(^{nd}\) order upwind scheme. A summary of numerical schemes used can be found in Table 3.4.

Hybrid simulations were run for 5 revolutions to allow the flow to reach a statistically steady periodic flow and sampled for at least 7 revolutions. Samples were taken every 90° of rotor rotation resulting in four samples per revolution. RANS simulations were similarly run for
5 revolutions to reach a statistically steady solution and sampled over the course of an additional 5 revolutions.

Table 3.4: Summary of numerical schemes for different turbulence models.

<table>
<thead>
<tr>
<th>Scheme</th>
<th>SBES</th>
<th>IDDES</th>
<th>KW-SST</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spatial Discretization</td>
<td>SIMPLC</td>
<td>SIMPLC</td>
<td>SIMPLE</td>
</tr>
<tr>
<td>Pressure</td>
<td>2nd Order</td>
<td>2nd Order</td>
<td>2nd Order</td>
</tr>
<tr>
<td>Momentum</td>
<td>Bounded Central Differencing</td>
<td>Bounded Central Differencing</td>
<td>2nd Order Upwind</td>
</tr>
<tr>
<td>Turbulent Kinetic Energy</td>
<td>2nd order Upwind</td>
<td>2nd order Upwind</td>
<td>2nd order Upwind</td>
</tr>
<tr>
<td>Specific Dissipation Rate</td>
<td>2nd order Upwind</td>
<td>2nd order Upwind</td>
<td>2nd order Upwind</td>
</tr>
</tbody>
</table>
Chapter 4: Results

4.1 Pressure Head Validation

Beginning the evaluation of turbulence models over the FDA Pump, Figure 4.1 displays the experimental and CFD pressure head rises across the 12 million cell and 19 million cell meshes for the RANS and Hybrid models respectively. The SBES model provides the most accurate predictions of pressure head where the IDDES model also predicts a slightly higher head rise, though within experimental error. Transient K-ω SST cases generally underpredict the experimental mean and underpredict the experimental range for test conditions 4 & 5.

![Graph showing averaged pressure head results in mmHg for simulated flow conditions]

Figure 4.1: Averaged pressure head results in mmHg for simulated flow conditions
4.2 Turbulent Kinetic Energy

In validating the mesh for LES regions, the resolved and turbulent TKE were computed and created and the percentage of the resolved TKE is depicted in Figure 4.2. In the boundary layer, the percentage of resolved TKE drops as the SBES and IDDES switch from their LES modes to the K-ω SST model. The SBES model shows an increased level of boundary layer shielding in the rotor region in comparison to the IDDES model indicating the IDDES model switching to WMLES mode and evaluating a larger portion of the boundary layer in LES. This difference in shielding can be observed in the diffuser region where flow separation leads to increased TKE on the resolved and SGS scales. The SBES boundary layer on the outside wall of the diffuser extends into the free stream of the diffuser leading to an increased level of SGS TKE generation as the K-ω SST model is used to simulate flow in this region. Between impellers, the SBES model shows a reduced level of sub-grid TKE compared to the IDDES model, which can be attributed to the differences in eddy viscosity computation between the two models.

Overall, both models confirm the mesh suitable for LES use where approximately 90% of TKE content is resolved by the mesh in the bulk flow. Due to a lack of experimental data for TKE, this aspect of the simulation cannot be appropriately validated. However, Derksen and Vanden Akker [72] similarly computed TKE and TKE dissipation in a Rushton turbine and determined that unvalidated dissipation computations were acceptable due to the relative accuracy of their TKE computations. Despite the lack of experimental TKE data, we believe our hybrid simulations are able to provide an accurate benchmark for both TKE and TKE dissipation due to the percent resolved TKE within the rotor.
4.3 Velocity Validation

Accounting for the unsteady flow of centrifugal pumps, particularly in the rotor and diffuser, velocity data was averaged over time for at least 7 revolutions of the pump impeller with four samples taken each revolution for a total of 28 samples per case. Figure 4.3 displays averaged contours for all cases.

In terms of general flow features, the SBES and IDDES models generally agree with each other for all cases. The K-ω SST agrees with hybrid model predictions within the rotor region, though predictions of the diffuser jet differ greatly. The K-ω SST model also appears to match the velocity increases at the cutwater for conditions 4 and 6 that the hybrid models see. For condition 1, all three models tend towards the inner wall of the diffuser with the K-ω SST model.
predicting a breakdown of the diffuser jet beyond the hybrid models. A similar trend is observed for conditions 4, 5 and 6 where the $K-\omega$ SST predicts a jet breakdown beyond the hybrid models while tending to the outside wall.

![Mean in-plane velocity contours](image)

Figure 4.3: Mean in-plane velocity contours. A-D: SBES conditions 1, 4, 5 and 6 respectively. E-H: IDDES conditions 1, 4, 5 and 6. I-L: $K-\omega$ SST conditions 1, 4, 5 and 6.

Within the rotor, both hybrid and RANS models show good agreement with PIV results for Q1 as seen in Figure 4.4. Near the wall however, all three CFD models predict a second peak in velocity observable for all conditions where experimental results show otherwise. This may be explained by the difficulty in capturing near-wall velocity gradients experimentally with PIV. Semenzin et al. [24] simulated the FDA blood pump using the SBES model and similarly reported a near wall velocity peak of near-identical magnitude for Q1. For condition 1, an
underprediction in the velocity of the rotor wake is seen for the K- ω SST though not observed in subsequent cases. Condition 6 proves to perhaps be the most challenging for the turbulence models examined as velocity of the impeller wake and near wall region is overpredicted by all three models. General trends overprediction of velocity in the wake region for Q1 may be explained by instabilities in the flow due to separation at the cutwater.

Figure 4.4: Time-averaged velocity profiles along quadrant 1. A: Condition 1, B: Condition 4, C: Condition 5, D: Condition 6

Similar velocity validation profiles for Q2 are seen in Figure 4.5. Again, the K- ω SST model is underpredicts portions of the impeller wake for condition 1, however this observation is not found for other cases. Overall, all three turbulence models show good velocity agreement.
Figure 4.5: Time-averaged velocity profiles along quadrant 2. A: Condition 1, B: Condition 2, C: Condition 5, D: Condition 6

Condition 5 was the only experimental flow condition with velocity data provided on the cutwater region attaching the rotor and outlet diffuser and is shown in Figure 4.6. Additional contours illustrating the magnitude difference between experimental and numerical results show large discrepancies in the cutwater and diffuser locations. Experimental results show the outlet jet for Condition 5 tends to the outside wall where both the SBES and IDDES models predict a more centrally located jet and a recirculation zone near the inner wall. The K-ω SST model predicts a profile similar to the experimental results where the outlet jet tends to the outside wall. Large differences in velocity magnitude are observed as the recirculation zone predicted by the
K-ω SST underpredicts velocity in the central portion of the diffuser and far overpredicts the overall velocity magnitude of the outlet jet.

Figure 4.6: A, B, C, D Time averaged velocity contours of PIV, SBES, IDDES, K-ω SST respectively for condition 5. E Time averaged velocity profile in diffuser at D4 in A. F, G, H Contours of velocity difference in SBES, IDDES, K-ω SST respectively.

Further information on the diffuser jet for condition 5 is provided in Figure 4.7. The general trend for the profile and magnitude are predicted well at the entrance of the diffuser for slice D1 across all three turbulence models, however the progression of the jet for the K-ω SST shows the gradual trend towards the wall. Both hybrid models show improved predictions on the breakdown of the turbulent jet with respect to both velocity and position. The primary difference between hybrid models can be identified at slice D4 where the jet is seen to break down faster in the IDDES model. Through the rotor, few differences between the K-ω SST and hybrid models are found, though velocity agreement across the diffuser is shown to be improved with the hybrid models. Additional figures for velocity validation within the diffuser can be found in Appendix B.
Figure 4.7: Diffuser profiles along D1-D4 (x = 0.02, 0.025, 0.03, 0.035 respectively) for condition 5. A: Experimental, B: SBES, C: IDDES, D: K-ω SST. Horizontal axis flipped.

4.4 Hemolysis Validation

4.4.1 Standard Power Law Model Results

Hemolysis was computed by implementing User Defined Scalars in Ansys Fluent and computing the scalar transport equations. The mass-weighted average of each scalar was recorded at the domain outlet. The scalars were then exponentiated by each power-law model’s respective β to calculate the HI%. The results for each case and simulation are shown in Figure 4.8 and presented as HI% for a single flowthrough of the pump.

From Figure 4.8, hemolysis is overpredicted by several orders of magnitude by all power law formulations. The hybrid EDS models compute slightly lower hemolysis values to their von
Mises stress counterparts whereas for the K-ω SST model, the EDS in the power-law results in an order of magnitude reduction from the total von Mises stress. Comparing relative trends of the power-law model across flow conditions, we find the Ding-Porcine hybrid model incorrectly predicts the trend in hemolysis between conditions 1 and 4 where experimental results show a decreasing rate of hemolysis with increasing flow rate at a constant RPM.

Figure 4.8: HI% results for EDS and von Mises stress against experimental results scaled to a single flow pass through the pump for all conditions.

Figure 4.9 presents the relative hemolysis index (RIH) for EDS based models and better presents relative hemolysis predictions by normalizing HI% to condition 5. It was observed by Taskin et al. that hemolysis decreases when the rotor speed of a blood pump is held constant and flow rate is increased. Fraser et al. also found hemolysis increases when rotor speed is increased at a constant flow rate. Both hybrid models are seen to predict the relative decrease in hemolysis for 2500RPM case as well as the increase between the 3500 RPM cases, however the predicted increase from condition 5 to condition 6 is several times lower than experimental results. The K-
ω SST models predict a rise in hemolysis in both the 2500 and 3500 RPM cases, however the Giersiepen and Ding-Porcine models accurately predict the decrease in hemolysis between increasing rotational rates at the same flow rates between conditions 4 and 5.

Figure 4.9: RIH case comparison. Hemolysis data presented as the ratio of one model and flow condition to the same model at condition 5: 6.0L/min, 3500RPM. Condition 5 used for normalization due to a measurable amount of hemolysis found during laboratory testing.

Table 4.1 presents a full set of relative HI% performance data for both EDS and von Mises stresses at constant rotational rates. With the exception of the Ding-Porcine models, the EDS results for the 2500 RPM cases reflect the relative decrease in hemolysis for the hybrid models and the noted increase in hemolysis for the 3500 RPM cases despite underpredicting the change by an order of magnitude. Most notably, the SBES GW VM and TZ VM models best predict the relative decrease between flow conditions at 2500 RPM within 2%. The IDDES EDS models generally predict the decrease at 2500 RPM with greater variance, however most von Mises models predict a positive change in hemolysis. Neither EDS nor von Mises stresses accurately predict the trend at 2500 RPM for the K-ω SST, though do come closest to the magnitude of change for the 3500 RPM conditions.
It should be noted that during preliminary laboratory tests for condition 6, intermittent cavitation was observed at the cutwater lip which may have contributed to an increase in hemolysis during experimentation. There is therefore a lack of confidence in the experimental data for this condition and relative hemolysis performance cannot be confidently compared for the 3500 RPM cases.

Table 4.1: Percent change in HI% at constant rotation rate. Experimental change at 2500 RPM was -12.5%. Experimental change at 3500 RPM was 232.1%.

<table>
<thead>
<tr>
<th>RPM</th>
<th>LPM</th>
<th>GW EDS</th>
<th>HO EDS</th>
<th>TZ EDS</th>
<th>DP EDS</th>
<th>GW VM</th>
<th>HO VM</th>
<th>TZ VM</th>
<th>DP VM</th>
</tr>
</thead>
<tbody>
<tr>
<td>2500</td>
<td>6</td>
<td>18.0%</td>
<td>8.2%</td>
<td>13.9%</td>
<td>10.6%</td>
<td>6.7%</td>
<td>2.3%</td>
<td>19.4%</td>
<td>19.9%</td>
</tr>
<tr>
<td>3500</td>
<td>6</td>
<td>6.7%</td>
<td>-21.8%</td>
<td>13.8%</td>
<td>25.3%</td>
<td>2.3%</td>
<td>19.4%</td>
<td>29.6%</td>
<td>20.5%</td>
</tr>
</tbody>
</table>

4.4.2 Threshold Power Law Model Results

Further evaluation of the power law models included evaluation of a simple scalar stress threshold at which no hemolysis occurs below with the SBES turbulence model and EDS power law model. As previous hemolysis experiments have investigated the stress threshold at which incipient hemolysis occurs, this incipient hemolysis has been investigated in this work. The threshold stress applied to the power law can be expressed as

$$HI\% = \begin{cases} C \tau^\alpha \tau^\beta, & \tau > \tau_{threshold} \\ 0, & \tau < \tau_{threshold} \end{cases}$$

(4.1)
Yen et al. [66] determined an EDS threshold at 50 Pa for a submerged jet which was evaluated in this study. Additionally, a 150 Pa threshold was tested to evaluate the sensitivity of the power law model. Taking initial HI% results as a baseline, Table 4.2 displays the percent decrease of HI between initial and threshold results.

Table 4.2: Percent decrease of HI% due to threshold stress effects.

<table>
<thead>
<tr>
<th>Test Condition</th>
<th>GW EDS</th>
<th>HO EDS</th>
<th>TZ EDS</th>
<th>DP EDS</th>
</tr>
</thead>
<tbody>
<tr>
<td>50 Pa Threshold</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C1</td>
<td>-4.33%</td>
<td>-9.44%</td>
<td>-4.11%</td>
<td>-0.21%</td>
</tr>
<tr>
<td>C4</td>
<td>-4.15%</td>
<td>-10.17%</td>
<td>-4.04%</td>
<td>-0.06%</td>
</tr>
<tr>
<td>C5</td>
<td>-1.98%</td>
<td>-5.27%</td>
<td>-1.95%</td>
<td>-0.04%</td>
</tr>
<tr>
<td>C6</td>
<td>-1.08%</td>
<td>-3.48%</td>
<td>-1.08%</td>
<td>-0.02%</td>
</tr>
<tr>
<td>150 Pa Threshold</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>C1</td>
<td>-39.40%</td>
<td>-55.07%</td>
<td>-36.45%</td>
<td>-4.66%</td>
</tr>
<tr>
<td>C4</td>
<td>-25.11%</td>
<td>-43.05%</td>
<td>-23.59%</td>
<td>-1.15%</td>
</tr>
<tr>
<td>C5</td>
<td>-17.36%</td>
<td>-29.22%</td>
<td>-16.10%</td>
<td>-0.90%</td>
</tr>
<tr>
<td>C6</td>
<td>-23.52%</td>
<td>-31.64%</td>
<td>-21.15%</td>
<td>-1.13%</td>
</tr>
</tbody>
</table>

We find that for the 50 Pa threshold, the HO model is the most sensitive to changes in stress. Decreases in HI% at this threshold are almost negligible with respect to experimental results. The 150 Pa threshold results in more significant decreases in HI%, however similar to the 50 Pa threshold, overall comparisons to experimental levels of hemolysis are several orders of magnitude off.

The relative performance across pump operating conditions was also evaluated. With the initial results as a baseline, it is observed that threshold power law models vary in their relative performance predictions. For the 50 Pa threshold, the GW model sees minor improvements towards experimental values. The HO model sees reduced performance between flow rates at the 2500 RPM operating points, however, sees an increase percent change with the 3500 RPM
operating points. The TZ model shows similar improvements to the GW model and the DP model sees relatively little change reflective of HI% change in Table 4.3.

Table 4.3: Percent change in HI% for threshold power law models at constant rotation rate. Experimental change at 2500 RPM was -12.5%. Experimental change at 3500 RPM was 232.1%.

<table>
<thead>
<tr>
<th>RPM</th>
<th>Flow Rate</th>
<th>GW EDS</th>
<th>HO EDS</th>
<th>TZ EDS</th>
<th>DP EDS</th>
</tr>
</thead>
<tbody>
<tr>
<td>0 Pa</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2500 RPM</td>
<td>2.5L/min</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>6.0L/min</td>
<td>-16.6%</td>
<td>-26.8%</td>
<td>-16.1%</td>
<td>22.8%</td>
</tr>
<tr>
<td>3500 RPM</td>
<td>6.0L/min</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>7.0L/min</td>
<td>18.0%</td>
<td>8.2%</td>
<td>13.9%</td>
<td>10.6%</td>
</tr>
<tr>
<td>50 Pa</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2500 RPM</td>
<td>2.5L/min</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>6.0L/min</td>
<td>-16.4%</td>
<td>-27.4%</td>
<td>-16.0%</td>
<td>23.0%</td>
</tr>
<tr>
<td>3500 RPM</td>
<td>6.0L/min</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>7.0L/min</td>
<td>19.1%</td>
<td>10.3%</td>
<td>14.9%</td>
<td>10.6%</td>
</tr>
<tr>
<td>150 Pa</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>2500 RPM</td>
<td>2.5L/min</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>6.0L/min</td>
<td>3.1%</td>
<td>-7.2%</td>
<td>0.9%</td>
<td>27.3%</td>
</tr>
<tr>
<td>3500 RPM</td>
<td>6.0L/min</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td>7.0L/min</td>
<td>9.2%</td>
<td>4.5%</td>
<td>7.1%</td>
<td>10.3%</td>
</tr>
</tbody>
</table>

The 150 Pa threshold sees markedly worse performance as the relative change at the 2500 RPM flow conditions show a positive increase in hemolysis for the GW and TZ models. The 3500 RPM flow conditions for the same models both see a decrease in change between flow rates as well. The HO model sees an increase in relative percent change closer resulting to a similar change to experimental values for the 2500 RPM flow conditions, a decrease in percent change is also seen at the 3500 RPM flow conditions. As with the 50 Pa threshold, the DP model sees relatively little change with respect to the stress threshold. Further analysis on the impacts of a stress threshold is covered in the following section.
4.5 Scalar Shear Stress Analysis

4.5.1 Von Mises and EDS Evaluation

Given the strong performance of the CFD models in the rotor region, shear stress fields can be taken as reasonably representative of the flow field in that region, however due to the lack of experimental data, direct comparisons cannot be made. In taking the hybrid model stress fields as a benchmark, we observe that the RANS model greatly overpredicts total stress in the rotor and diffuser regions as seen in Figure 4.10. Figure 4.11 illustrates shear stress contours of the Reynolds and viscous stresses of the K-ω SST model against the total stress evaluated by the Hybrid models across the Q1 line.

Figure 4.10: Contours of total von Mises and EDS for condition 5. A, B, C Contours of SBES total von Mises stress, IDDES total von Mises stress, K-ω SST total von Mises stress respectively. D, E, F Contours of total EDS of SBES, IDDES, K-ω SST.
We find for the K-ω SST model, viscous stress underpredicts the general stress profile along the Q1 radial profile as opposed the Hybrid models. We additionally observe that the von Mises stress profile resembles the resolved stresses of the LES regions in the hybrid models with a magnitude approximately an order of one magnitude lower.

Figure 4.11: Total hybrid von Mises stress vs K-ω SST component stress profiles for condition 5. A, B von Mises stress and EDS along quadrant 1. C, D Component stress along quadrant 2. E, F Component stress along diffuser.

In examining the EDS profiles, we find the RANS model in better agreement with the Hybrid models. Figure 4.11 shows that the RANS EDS across the rotor is about the same level of magnitude as the hybrid models with following. With respect to the EDS profile across the rotor, the RANS model tends to predict EDS levels in line with the Hybrid models with slight overpredictions in magnitude following the wake of the impeller. The hybrid models also
similarly agree within the outlet diffuser with to EDS where the RANS model also lies within the same order of magnitude.

The volume average of stresses through the rotor partition in the computational domain are shown in Figure 4.12 illustrating the difference in magnitude between stresses across flow conditions and turbulence models. As expected, stresses for both SBES and IDDES models are similar in magnitude across all flow conditions and total von Mises stress for the K-ω SST model are multiple times larger than that of the hybrid models. We find Reynolds stresses contribute the most in terms of magnitude to the total stress tensor. Comparatively, the ratio of viscous stress to Reynolds stress in Table 4.4 is an order of magnitude lower than the ratio for resolved stress to SGS stress indicating a severe overprediction of Reynolds stresses through the computational domain. From this, it may be suitable to say the Reynolds stress may not be an accurate metric to use within the power law model.

![Figure 4.12: Volume average of scalar stresses within the rotor domain.](image)
Table 4.4: Ratio of resolved to SGS stress in hybrid models and ratio of viscous to Reynolds stress in the K-ω SST model within the rotor partition.

<table>
<thead>
<tr>
<th>Condition</th>
<th>1</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>SBES</td>
<td>5.38</td>
<td>4.15</td>
<td>2.87</td>
<td>2.78</td>
</tr>
<tr>
<td>IDDES</td>
<td>4.60</td>
<td>3.18</td>
<td>2.59</td>
<td>2.43</td>
</tr>
<tr>
<td>K-ω SST</td>
<td>0.32</td>
<td>0.21</td>
<td>0.17</td>
<td>0.16</td>
</tr>
</tbody>
</table>

The volume average of EDS computed with the K-ω SST model correlates well with the EDS of the hybrid models. Table 4.5 displays the relative percentage increase of the SBES and IDDES models from the K-ω SST model stresses. We find the percent increase of EDS through the rotor partition is an order of magnitude lower than the von Mises stresses indicating that the K-ω SST predicts overall energy dissipation well compared to the hybrid models as a baseline.

Table 4.5: Relative increase in percent of K-ω SST total EDS and von Mises stress to hybrid total EDS and von Mises stresses within the rotor domain.

<table>
<thead>
<tr>
<th>Condition</th>
<th>1</th>
<th>4</th>
<th>5</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>SBES EDS</td>
<td>10.1%</td>
<td>20.7%</td>
<td>24.0%</td>
<td>27.5%</td>
</tr>
<tr>
<td>IDDES EDS</td>
<td>13.5%</td>
<td>22.1%</td>
<td>29.7%</td>
<td>34.6%</td>
</tr>
<tr>
<td>SBES Total VM</td>
<td>126.0%</td>
<td>185.8%</td>
<td>211.8%</td>
<td>228.8%</td>
</tr>
<tr>
<td>IDDES Total VM</td>
<td>127.2%</td>
<td>175.9%</td>
<td>214.9%</td>
<td>233.7%</td>
</tr>
</tbody>
</table>

From this analysis, it is strongly suggested that an energy dissipation based hemolysis model may lead to a unified framework to predict hemolysis across turbulence model types. We find, despite differences in energy dissipation distribution, the volume average dissipation scalar stress for the K-ω SST model within the rotor region was found to be similar in magnitude to the hybrid models and is reflected in the resultant HI%. Given that the contributions of Reynolds and viscous stresses are at the extremes of the total stress contribution, it is doubtful that either Reynolds or viscous scalar shear stresses should be used as an effective stress for the power-law model.
4.5.2 Hemolysis Damage Index and Stress Influences

Visualization of blood damage and associated stresses allows for the identification of flow regions with the potential to cause blood damage. The scalar damage index (DI) computed as $H'$ in Equation 2.70 allows for visualization of hemolysis generation and convection through the computational domain. Figure 4.13 displays the DI for the Giersiepen power law model and corresponding scalar EDS field for each flow condition simulated by the SBES model.

DI is seen to be relatively constant through the rotor region, however a high concentration of DI is seen at the pump cutwater at conditions 4, 5 and 6. Visualization of EDS shows high stresses on the inside and outside walls of the diffuser; however, the leading edge of the cutwater appears to generate the highest DI. From Figure 4.3, CFD predictions for conditions 4, 5 and 6 either show diffuser jets tending to the center or outside wall of the diffuser whereas the outlet jet for condition 1 tends towards the inside wall. This indicates that high stresses due to flow separation in this region may be greatly influenced by cutwater design.

Large von Mises stresses as seen in Figure 4.10 and EDS in Figure 4.13 located in the constricted outlet piping between the cutwater and diffuser can be attributed to an increase in velocity in the same region seen in Figure 4.3. The flow constriction leads to a reduction in pressure and corresponding velocity increase due to Bernoulli’s principle where shear stresses increase near the wall due to larger velocity gradients. Additionally, the leading edge of the cutwater acts like an airfoil in creating a low pressure, high velocity region further contributing to the acceleration of fluid through the outlet.

In recovering pressure loss by the constriction, the diffuser increases the outlet pipe diameter, reducing the velocity and increasing pressure. The resulting turbulent jet produces increased EDS and von Mises stresses within the diffuser as seen in Figure
Due to the highest velocities of the outlet jets tending towards the outside wall for conditions 4, 5 and 6, we can generally see larger magnitudes of both, EDS and von Mises stress produced along the outside wall of the diffuser as well. As mentioned previously, EDS computations predict lower magnitudes of shear stresses than their von Mises counterparts, however the spatial locations of the scalar stresses closely mirror each other.

![Figure 4.13: Instantaneous scalar damage index (DI) and associated EDS contours of the SBES model. A-D: DI contours of condition 1, 4, 5 and 6. E-H: EDS contours of condition 1, 4, 5 and 6.](image)

As the FDA blood pump was designed to generally resemble centrifugal blood pumps and their characteristic features, it may be helpful to contextualize the results of this work with respect to industrial designs. The HeartMate 3 (HM3, Abbott, St. Paul, MN, USA) is one of the latest devices to be released on the market aiming to provide long-term support to patients with
advanced heart failure. Thamsen et al. [14] conducted CFD simulations validated by 3D-PTV measurements of the HM3 at flow rates of 2.7 and 5.7 L/min at a rotation rate of 5000 RPM. Obvious geometric differences between the FDA pump and the HM3 can be seen with the pump housing leading to a constant diameter outlet pipe as well as impeller design.

Figure 4.14: Instantaneous EDS and von Mises stress contours for conditions 1-6, SBES model. A-D: Conditions 1, 4, 5 and 6 EDS contours respectively. E-H: Conditions 1, 4, 5 and 6 EDS contours respectively.

Comparing the 5.7L/min flow condition of the HM3 to condition 5 (6L/min, 3500 RPM) of the FDA pump, mean velocity contours of the HM3 along three different sectional planes show relatively constant velocities across each plane from the impellers to the outlet [14]. The FDA pump experimentally and computationally show large velocity gradients across the rotor domain and through the outlet diffuser. Additionally, TKE was found to have relatively low variance across streamlines from the impellers to the outlet for the HM3 whereas high regions of TKE can be easily identified trailing the impeller blades and diffuser for the FDA pump in Figure 4.2. From this observation, it can be said that mechanical energy imparted to fluid in the
HM3 is better conserved than the FDA pump resulting in less energy dissipation and potentially, lower hemolysis generation. Additionally, streamlines show reduced flow separation at the cutwater indicating the cutwater is better optimized for the observed operating conditions than the FDA pump.

4.5.3 Threshold Stress

The effect of a simple stress threshold mentioned previously results in relatively small reductions in HI%. Although the largest reduction reaches up to 55%, experimental results still show several orders of magnitude difference in hemolysis results. Contours illustrating the influence of a stress threshold on the power law model are displayed in Figure 4.15. Between the zero threshold and 50 Pa threshold cases, minimal difference is seen between DI contours. Stress contours show immediate reduction in the spatial distribution stresses between baseline and 50 Pa threshold cases.

Drastic reductions in the applied stress are seen in the 150 Pa threshold case, however computed hemolysis does not decrease appreciably. The DI contour for the 150 Pa threshold case shows that DI is still of a similar level to the baseline and 50 Pa threshold cases in the rotor region indicating hemolysis is generated near the rotor walls with high velocity gradients. Notably, stresses for the 150 Pa case are isolated to small regions following the cutwater and parallel wall where fluid is seen to accelerate due to flow area constriction. DI generated in the diffuser is greatly decreased as a result, indicating the design of the diffusor and cutwater regions are large contributors to hemolysis in the FDA pump.

Finally, analysis of contour plots with a high stress threshold indicates that a majority of stress in the bulk flow that would normally be considered damaging to RBCs are disregarded implying that this approach with the power law models is not feasible. Additionally, this
demonstration of a simple threshold stress demonstrates that the current power law models are unsuitable for use with this centrifugal pump design as stress cutoffs do not affect resultant HI% in a meaningful way. Power law coefficients may need to be regressed for different geometries and flow types to compute HI% values to resemble experimental results.

Figure 4.15: SBES condition 6 GW EDS DI and corresponding EDS contours of hemolysis threshold results. A-C: 0 Pa, 50 Pa and 150 Pa threshold DI contours respectively. D-E: 0 Pa, 50 Pa and 150 Pa threshold EDS contours respectively.

4.6 Discussion

This study is not the first to utilize hybrid RANS-LES models on the FDA blood pump, however to the author’s knowledge, is the first to comparatively study the differences in hemolysis between hybrid and RANS models on the FDA blood pump. Gross-Hardt et al. [23] was the first to apply the SBES model to the FDA blood pump in a study analyzing pressure, velocity and shear stress dependency on mesh quality. More recently, Semezin et al. [24]
similarly used the SBES model in a study proposing standardized guidelines for the usage of CFD in simulating centrifugal blood pumps. In the vein of higher resolution simulations of the FDA blood pump, Huo et al. [25] utilized a “Light LES” technique where under-resolved meshes and large time steps were shown to better capture mean flow, pressure and transient effects more effectively than URANS simulations. Common factors between all three studies include tetrahedral meshes with cell counts ranging from 8.26 to 24.7 million cells and time steps ranging from 5° of rotation per time step to 0.375° per time step. Comparatively, this study used a poly-hexacore mesh of 19.1 million cells with a time step equivalent to 0.225° of rotation per time step. Utilizing a hybrid structured mesh with a mixture of prism and hexahedral elements, the mesh in this study provides a more accurate solution than unstructured tetrahedral meshes of similar cell counts [73]. Additionally, the refined temporal resolution of the simulations in this work ensures the resolution of eddies to the limit of the computational grid.

In review of hemolysis predictions for the FDA blood pump, we found inconsistencies in the comparison of CFD and experimental results of similar works. The Eulerian power law model implies the resultant HI% is the change in hemolysis after a volume of blood equivalent to the volume in the experimental test circuit has passed through scaled by hematocrit [52]. This explicitly requires comparative experimental results to be similarly scaled to a single volumetric flow through of an experimental circuit in addition to hematocrit. Avci et al. [74] reports experimental results of the FDA blood pump as the ratio of pfHb to Hb normalized by hematocrit only. Good and Manning [75] reported power law pfHb values alongside experimental pfHb results implying the Giersiepen model provides a good fit to experimental data however, their NIH values are inconsistent with their reported pfHb. In recalculating the HI% from their pfHb and assumed Hb, we find their results with the Heuser Opitz coefficient similar to ours for the K-
SST turbulence model, however a simple conversion to NIH shows both models to be orders of magnitude away from the reported NIH. Wu et al [76], [77]. were the only group to report hemolysis results comparing power law models to experimental results by the appropriate normalization mentioned prior.

It should also be reiterated that despite experimental correlations between EDS and hemolysis [66], the mechanism at which lysis occurs in turbulent flows is still unknown though the hypothesis that Kolmogorov scale eddies the size of RBCs imparting dissipative energy on RBCs has spawned new empirical models for hemolysis. Ozturk et al. [78] used CFD simulations to directly correlate Kolmogorov scale eddies experimental hemolysis results later developed an empirical model [79] applied by Avci et al. [74] to the FDA blood pump. Tobin and Manning developed a EDS power law model accounting for intermittent SGS dissipation in a LES simulation of the FDA nozzle [21]. Wu et al. [77] regressed data from Boehning et al. [80] to develop an Eularian energy dissipation based model resulting in the closest agreement to the FDA blood pump data.

Finally, most CFD studies evaluating hemolysis typically model a homogenous fluid. To create a fully comprehensive model for hemolysis, cell-cell interactions must be considered in a continuous damage model which would have implications on both macro fluid properties and micro-scale flows between RBCs [81]. Discrete two-way coupled CFD simulations modeling RBC deformation with tools such as Hemocell may help provide insight into cell-cell interactions in various flow conditions [82]. Additionally, particle seeded DNS may also shed light on how energy in turbulent flows is affected by particles. Schneiders et al. [83] found that particles at the Kolmogorov scale absorb energy from the bulk flow and increase local dissipation as a result of high strain rates near particle surfaces which may have implications for
future developments in dissipation based hemolysis models. Insights from these techniques may help mature novel hemolysis modeling approaches.

4.7 Limitations

Although the simulations in this work resolve flow characteristics well, further experimental validation data is needed. As PIV data only provides velocity magnitude, velocity component data would be helpful in validating both stress and energy dissipation fields. In this study, stress and energy dissipation fields from hybrid models were used as a comparative benchmark for the K-ω SST model and highlight relative differences rather than absolute differences. As hybrid models utilize the K-ω SST model for near wall flows, comparative differences in these regions were not discussed. Additionally, these simulations utilized a Newtonian fluid model. A more accurate hemodynamic model may seek to incorporate a shear thinning or viscoelastic model.

For hemolysis predictions, the power law model coefficients used are regressed from laminar flow experiments and are limited to a range of shear stresses surpassed by a centrifugal pump. Recalibration of coefficients for the power law is needed for more accurate predictions in turbulent flow. Due to the near wall use of the K-ω SST model in the hybrid models, generation and convection of the damage scalars may be influenced by the turbulence model switch in these regions as well as flow inaccuracies inherent in the underlying RANS model.
Chapter 5: Conclusions

In accurately simulating the hemodynamics of blood pumps, thorough validation should be conducted. Outlet pressure for hybrid models agree well with experimental results for all conditions where the K-ω SST underpredicts experimental range for two of four conditions. Velocity predictions show good agreement for all models in the rotor region, though possess a higher velocity peak near the wall relative to experimental data. Additional hybrid models from literature, however, agree with these results. In the diffuser region, hybrid models show improvement over the K-ω SST in velocity predictions of the turbulent jet. The resolved turbulent kinetic energy content was computed and found that 80-90% of the kinetic energy was resolved spatially indicating that analysis concerning dissipation of energy may be held as an appropriate baseline for comparison to K-ω SST results of dissipation.

This study found that Reynolds stresses are the largest contributor to the total stress for the K-ω SST model resulting in hemolysis calculations an order of magnitude larger than the total stress for hybrid models and EDS for both models. Stress profiles through the rotor and diffuser show that EDS in the K-ω SST model provide good agreement with EDS computed by hybrid models in the rotor and diffuser relative to the total stress profiles. Profiles for the Reynolds stress severely overpredict the total stress seen in hybrid simulations and viscous stress conversely underpredicts the total stress. EDS for the K-ω SST model is seen to correlate well with hybrid model predictions in both volume average stress and stress profiles through the domain. It thus recommended that neither viscous nor Reynolds stress are used in the computation of hemolysis with the power law models and encourages further efforts in
continuum modeling of hemolysis in the context of dissipation and micro-scale turbulent effects as EDS or otherwise.

Furthermore, the effects of a simple stress threshold were analyzed for the power law model. In comparison to cases without a threshold stress, relative hemolysis predictions between flow conditions at constant rotation rates and constant flow rates worsened. Additionally, damage index contours show that threshold stress has little impact on hemolysis generation within the rotor domain indicating the power law model primarily generates hemolysis in near wall regions. Finally, analysis of contour plots with a high stress threshold indicates that a majority of stress in the bulk flow that would normally be considered damaging to RBCs are disregarded indicating that this approach with the power law models may not be accurate.
References


[73] M. Sosnowski, J. Krzywanski, and R. Gnatowska, “Polyhedral meshing as an innovative approach to computational domain discretization of a cyclone in a fluidized bed CLC


Appendix A: Sample Power Law UDF Code

```c
1. #include "udf.h"
2. #include<stdio.h>
3. #include<stdlib.h>
4. 
5. #define C_GW 0.0000363
6. #define alpha_GW 2.416 randy tran
7. #define beta_GW 0.785
8. 
9. #define C_HO 0.00018
10. #define alpha_HO 1.991
11. #define beta_HO 0.765
12. 
13. #define C_TZ 0.00001228
14. #define alpha_TZ 1.9918
15. #define beta_TZ 0.6606
16. 
17. #define C_DP 0.0006701
18. #define alpha_DP 1.0981
19. #define beta_DP 0.2778
20. 
21. #define prin_stress_size 3 // size of principal stress solution array
22. #define pi 3.1415926535897932384626433
23. 
24. #define turb_diss_mod_const 0.09
25. 
26. 
27. DEFINE_ADJUST(BD0,d)
28. {
29.     Thread *c_t;
30.     cell_t c;
31.     real mu;
32.     real tau11, tau22, tau33, tau12, tau23, tau13;
33.     real re_tau11, re_tau22, re_tau33, re_tau12, re_tau23, re_tau13;
34.     real tot_tau11, tot_tau22, tot_tau33, tot_tau12, tot_tau23, tot_tau13;
35. ```
int principal_stress_calc(double* sol_val, double* stress_array, int size) {
    /* Solving characteristic cubic equation using Cardan's Method */
    /* Since the stress tensor is a symmetric tensor whose elements are all real, it has real eigenvalues. That is, the three principal stresses are real */
    /* Input array::: real stress_array[]= {tau11, tau22, tau33, tau12, tau23 ,tau13 } */
    /* Local variable declaration */
    double p, q, r, I1, I2, I3, theta, sigma1, sigma2, sigma3;
    /* Invariants */
    I1 = -(stress_array[0] + stress_array[1] + stress_array[2]);
    //printf("I1 = %f\n", I1);
    //printf("I2 = %f\n", I2);
    //printf("I3 = %f\n\n\n\n", I3);
    /* p, q substitution values */
    p = I2 - (pow(I1, 2) / 3);
    //printf("P = %f\n", p);
    q = 2 * pow(I1, 3) / 27 - I1 * I2 / 3 + I3;
    //printf("Q = %f\n", q);
    /* solve for discriminant */
    r = sqrt(pow(-p, 3) / 27);
    /* If statement to prevent NaN*/
    /* 1/r term in theta calculation will cause inf error and crash program */
if (r == 0) {
    theta = 0;
    sigma1 = 0;
    sigma2 = 0;
    sigma3 = 0;
    sol_val[1] = 0;
    sol_val[1] = 0;
    sol_val[1] = 0;
}
else {
    theta = acos((-q / 2) * (1 / r));
    sigma1 = 2 * pow(r, 1.0 / 3.0) * cos(theta / 3) - I1 / 3;
    sigma2 = 2 * pow(r, 1.0 / 3.0) * cos((2 * pi + theta) / 3) - I1 / 3;
    sigma3 = 2 * pow(r, 1.0 / 3.0) * cos((4 * pi + theta) / 3) - I1 / 3;
    double max1 = MAX(sigma1, sigma2);
    double max2 = MAX(max1, sigma3);
    sol_val[0] = max2;
    // compute min
    double min1 = MIN(sigma1, sigma2);
    double min2 = MIN(min1, sigma3);
    sol_val[2] = min2;
    sol_val[1] = -I1 - sol_val[0] - sol_val[2];
}
return 0;

double tresca_criterion(double stresses[]) {
    /* Local variable declaration */
    double tau_tresca_criterion, max1, max2;
    /* Computing maximum sigma difference */
    max1 = MAX(pow(stresses[0] - stresses[1], 2),
        pow(stresses[1] - stresses[2], 2));
    max2 = MAX(max1, pow(stresses[0] - stresses[2], 2));
    tau_tresca_criterion = .5 * sqrt(max2);
    return tau_tresca_criterion;
}
double von_mises_criterion(double stress_array[]) {
    /* Input array::: real stress_array[] = {tau11, tau22, tau33, tau12, tau23, tau13} * /
    /* Local variable declaration */
    double term_1, term_2, term_3, term_4, von_mises_stress;

    /* Segmented calculation of Von Mises stress*/
    term_1 = pow(stress_array[0] - stress_array[1], 2);
    term_2 = pow(stress_array[1] - stress_array[2], 2);
    term_3 = pow(stress_array[2] - stress_array[0], 2);
    term_4 = 6 * (pow(stress_array[3], 2) + pow(stress_array[4], 2) + pow(stress_array[5], 2));
    von_mises_stress = sqrt(.5 * (term_1 + term_2 + term_3 + term_4));

    //printf("\nIn-function calculation of Von Mises\n");
    //printf("Von Mises Stress = %f\n", von_mises_stress);

    return von_mises_stress;
}

thread_loop_c(c_t, d) {
    begin_c_loop(c, c_t) {
        mu = 0.0035;

        /* Begin viscous stress calculation */
        tau11 = 2 * C_DUDX(c, c_t) * mu;
        tau22 = 2 * C_DVDY(c, c_t) * mu;
        tau33 = 2 * C_DWDZ(c, c_t) * mu;
        tau12 = (C_DUDY(c, c_t) + C_DVDX(c, c_t)) * mu;
        tau23 = (C_DVDZ(c, c_t) + C_DWDY(c, c_t)) * mu;
        tau13 = (C_DUDZ(c, c_t) + C_DWDX(c, c_t)) * mu;

        /* Input array::: real stress_array[] = {tau11, tau22, tau33, tau12, tau23, tau13} * /
/* Initialize output array principal stress*/
double visc_prin_stress[3]; // empty solution array

/* Call Principal Stress function*/
Calling back function
// Fills empty solution array
principal_stress_calc(visc_prin_stress, visc_stress_array, prin_stress_size);

// VM arg(flow field stress array)
// Return Von Mises
double tau_vm =
  von_mises_criterion(visc_stress_array);

// tresca_criterion arg(solution array, principal stress)
// Return Tresca
double tau_tresca =
  tresca_criterion(visc_prin_stress);

// Store in cell memory before function overwritten
C_UDMI(c, c_t, 0) = tau_vm/sqrt(3);
C_UDMI(c, c_t, 1) = tau_tresca;
/* End viscous stress calculation*/

/* Begin reynolds stress calculation for incompressible flow */
// See Boussinesq eddy viscosity assumption
// kroniker delta = 1 if i==j
re_tau11 = 2*(C_DUDX(c,c_t))*C_MU_T(c,c_t) - 2/3*C_R(c,c_t)*C_K(c,c_t);
re_tau22 = 2*(C_DVDY(c,c_t))*C_MU_T(c,c_t) - 2/3*C_R(c,c_t)*C_K(c,c_t);
re_tau33 = 2*(C_DWDZ(c,c_t))*C_MU_T(c,c_t) - 2/3*C_R(c,c_t)*C_K(c,c_t);
re_tau12 = C_MU_T(c,c_t) * (C_DUDY(c,c_t) + C_DVDX(c,c_t));
re_tau23 = C_MU_T(c,c_t) * (C_DVDZ(c,c_t) + C_DWDY(c,c_t));
re_tau13 = C_MU_T(c,c_t) * (C_DUDZ(c,c_t) + C_DWDX(c,c_t));
double reynolds_stress_array[6] = { re_tau11, re_tau22, re_tau33, re_tau12, re_tau23, re_tau13 }; // empty solution array

principal_stress_calc(reynolds_prin_stress, reynolds_stress_array, prin_stress_size);

double re_tau_vm = von_mises_criterion(reynolds_stress_array);

double re_tau_tresca = tresca_criterion(reynolds_prin_stress);

C_UDMI(c, c_t, 2) = re_tau_vm/sqrt(3);
C_UDMI(c, c_t, 3) = re_tau_tresca;

/* End reynolds stress calculation */

/* Begin total stress calculation for incompressible flow */

tot_tau11 = tau11 + re_tau11;
tot_tau22 = tau22 + re_tau22;
tot_tau33 = tau33 + re_tau33;
tot_tau12 = tau12 + re_tau12;
tot_tau23 = tau23 + re_tau23;
tot_tau13 = tau13 + re_tau13;

double tot_stress_array[6] = { tot_tau11, tot_tau22, tot_tau33, tot_tau12, tot_tau23, tot_tau13 }; // empty solution array

principal_stress_calc(tot_prin_stress, tot_stress_array, prin_stress_size);

double tot_tau_vm = von_mises_criterion(tot_stress_array);

double tot_tau_tresca = tresca_criterion(tot_prin_stress);

C_UDMI(c, c_t, 4) = tot_tau_vm/sqrt(3);
C_UDMI(c, c_t, 5) = tot_tau_tresca;

/* End total stress calculation for incompressible flow */
// Compute RANS Energy Dissipation
real rans_diss = C_O(c,c_t)*C_K(c,c_t)*0.09;

C_UDMI(c, c_t, 6) = rans_diss;
C_UDMI(c, c_t, 7) = pow(C_UDMI(c, c_t, 6) * 0.0035 * C_R(c, c_t), 0.5);

real resolved_diss = mu * pow(C_STRAIN_RATE_MAG(c,c_t), 2)/C_R(c,c_t);
real subgrid_diss = C_MU_T(c, c_t)*pow(C_STRAIN_RATE_MAG(c, c_t), 2)/ C_R(c, c_t);
real total_eds = resolved_diss + rans_diss;
real total_eds_stress = pow(total_eds * 0.0035 * 1035, .5);

C_UDMI(c, c_t, 8) = resolved_diss;
C_UDMI(c, c_t, 9) = total_eds;
C_UDMI(c, c_t, 10) = pow(C_UDMI(c, c_t, 9) * 0.0035 * C_R(c, c_t), .5);

// C_D does not work in K-w model. Epsilon not directly calculated
// 0.09*k*w is equivalent formula to epsilon in K-w

C_UDMI(c, c_t, 0) = tau_vm;
C_UDMI(c, c_t, 1) = tau_tresca;
C_UDMI(c, c_t, 2) = re_tau_vm;
C_UDMI(c, c_t, 3) = re_tau_tresca;
C_UDMI(c, c_t, 4) = tot_tau_vm;
C_UDMI(c, c_t, 5) = tot_tau_tresca;
C_UDMI(c, c_t, 6) = rans_diss;
C_UDMI(c, c_t, 7) = pow(C_UDMI(c, c_t, 6) * 0.0035 * C_R(c, c_t), 0.5);
C_UDMI(c, c_t, 8) = resolved_diss;
C_UDMI(c, c_t, 9) = total_eds;
C_UDMI(c, c_t, 10) = pow(C_UDMI(c, c_t, 9) * 0.0035 * C_R(c, c_t), .5);

// end_c_loop(c,c_t)
/* Def VM source terms total stress, visc + reynolds */

C_UDMI(c, c_t, 4) /*

/* If you read this far, email me at jdtarriela@gmail.com */
/* Subject: Free beer-thesis easter egg*/
/* I’ll send you money for a case of beer*/
/* If you're digging this far for code, I bet you need one*/
/* Cheers! */

DEFINE_SOURCE(GW_vm_tot, c, t, dS, eqn)
{
    real C_term, Teff_term, source;
    C_term = pow(C_GW, 1.0/beta_GW);
    Teff_term = pow(C_UDMI(c, t, 4), alpha_GW / beta_GW);
    source = C_term * Teff_term * C_R(c, t);
    dS[eqn] = 0;
    return source;
}

DEFINE_SOURCE(HO_vm_tot, c, t, dS, eqn)
{
    real C_term, Teff_term, source;
    C_term = pow(C_HO, 1.0/beta_HO);
    Teff_term = pow(C_UDMI(c, t, 4), alpha_HO / beta_HO);
    source = C_term * Teff_term * C_R(c, t);
    dS[eqn] = 0;
    return source;
}

DEFINE_SOURCE(TZ_vm_tot, c, t, dS, eqn)
{
    real C_term, Teff_term, source;
    C_term = pow(C_TZ, 1.0/beta_TZ);
    Teff_term = pow(C UDMI(c, t, 4), alpha_TZ / beta_TZ);
    source = C_term * Teff_term * C_R(c, t);
return source;
}

DEFINE_SOURCE(DP_vm_tot, c, t, dS, eqn) {
  real C_term, Teff_term, source;
  C_term = pow(C_DP, 1.0/beta_DP);
  Teff_term = pow(C_UDMI(c, t, 4), alpha_DP / beta_DP);
  source = C_term * Teff_term * C_R(c, t);
  return source;
}

/* ---------------------------------------------------------- */
/* Def source terms eds */ /* C_UDMI(c, c_t, 6) */
/* ---------------------------------------------------------- */
DEFINE_SOURCE(GW_eds, c, t, dS, eqn) {
  real C_term, Teff_term, source;
  C_term = pow(C_GW, 1.0/beta_GW);
  Teff_term = pow(C_UDMI(c, t, 10), alpha_GW / beta_GW);
  source = C_term * Teff_term * C_R(c, t);
  return source;
}

DEFINE_SOURCE(HO_eds, c, t, dS, eqn) {
  real C_term, Teff_term, source;
  C_term = pow(C_HO, 1.0/beta_HO);
  Teff_term = pow(C_UDMI(c, t, 10), alpha_HO / beta_HO);
  source = C_term * Teff_term * C_R(c, t);
  return source;
}
DEFINE_SOURCE(TZ_ed, c, t, dS, eqn) {
    real C_term, Teff_term, source;
    C_term = pow(C_TZ, 1.0/beta_TZ);
    Teff_term = pow(C_UDMI(c, t, 10), alpha_TZ / beta_TZ);
    source = C_term * Teff_term * C_R(c, t);
    return source;
}

DEFINE_SOURCE(DP_ed, c, t, dS, eqn) {
    real C_term, Teff_term, source;
    C_term = pow(C_DP, 1.0/beta_DP);
    Teff_term = pow(C_UDMI(c, t, 10), alpha_DP / beta_DP);
    source = C_term * Teff_term * C_R(c, t);
    return source;
}
Appendix B: Velocity Validation Plots

Figure B.1: Diffuser jet profiles condition 1. A: Experimental. B: SBES. C: IDDES. D: K-ω SST
Figure B.2: Diffuser jet profiles condition 6. A: Experimental. B: SBES. C: IDDES. D: K-ω SST

Figure B.3: Instantaneous velocity contours for condition 5. A: SBES, B: IDDES, C: K-ω SST