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PREDICTION OF THE HYDRODYNAMICS IN STIRRED TANK REACTORS

by

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Thesis presented for the degree of Master of Science in Engineering
in the Department of Chemical Engineering
University of Cape Town

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PLAGIARISM DECLARATION

I know the meaning of plagiarism and declare that all the work in the document, save for that which is properly acknowledged, is my own.

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I express my unreserved gratitude to God for His love, faithfulness and wisdom throughout the research. This piece of work is dedicated to Him.

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NOMENCLATURE

T	tank diameter	m
H	liquid level in the tank	m
C	impeller clearance	m
D	impeller diameter	m
d_h	hub diameter	m
w_b	blade width	m
l_b	blade length	m
d	disc diameter	m
$C_{\varepsilon_1}, C_{\varepsilon_2}, C_{\mu}$	turbulence model parameters in equations 2.20 – 2.24	-
S	modulus of the mean rate of strain tensor	-
P	pressure	Pa
$\bar{u}_i, u_j$	mean velocity components	m/s
$u'_i u'_j$	fluctuating velocity components	m/s
x_i, x_j	cartesian co-ordinates	m
S_{ϕ}	Source term in equations 2.3 and 2.12	-
g_i	gravitational acceleration in ith direction	m/s ²
u^+	dimensionless mean velocity profile assumed close to the wall	-
y^+	dimensionless distance from the wall	-
B	empirical constant related to the thickness of the viscous sub-layer	-
U	axial velocity	m/s
V	radial velocity	m/s
W	tangential velocity	m/s
k	turbulent kinetic energy	m ² /s ²
Z	axial coordinate	m
Re	Reynolds number	-
N	impeller rotational speed	rpm
U_{tip}	impeller tip speed	m/s

$\vec{r}_{AB}$	moment vector	m
$\vec{F}_p$	pressure force vector	N
$\vec{F}_v$	viscous force vector	N
M	torque	Nm
N_p	power number	-
P_0	power consumption	W
Pe	Peclet number	-
$U_{\text{error}}, V_{\text{error}},$ W_{error}	Error values for the normalised mean velocities	-
K_{error}	Error value for the normalised turbulent kinetic energy	-

Greek symbols

ε	dissipation rate of turbulent kinetic energy	m^2/s^3
$\sigma_\varepsilon, \sigma_k$	effective turbulent Prandtl numbers for the transport of ε and k .	-
ρ	density	kg/m^3
κ	Von karman constant	-
μ_t	eddy viscosity	kg/ms
μ_{eff}	effective viscosity	kg/ms
ω	specific dissipation rate	
α	constant in $k - \omega$ model	-
ν_t	kinematic eddy viscosity	m^2/s
ν	kinematic molecular viscosity	m^2/s
ϕ	scalar quantity that represent either temperature or species concentration in equations 2.3 and 2.12	-
λ	diffusivity of ϕ	
$\alpha, \beta^*, \beta, \sigma, \sigma^*$	constants in $k - \omega$ model	-
β, η	constants in RNG $k - \varepsilon$ model	-
σ_{est}	standard error of estimate	-

g	turbulent velocity scale	m/s
ℓ	length scale	m
ℓ_m	Prandtl mixing	m
ϕ	dependent flow variable	
Γ_ϕ	diffusion coefficient	-
δx	cell size	-

Subscripts

i,j,k	Directional coordinates
---------	-------------------------

Abbreviation

CFD	Computational Fluid Dynamic
MFR	Multiple Frame of Reference
SG	Sliding Grid
IBC	Impeller Boundary Condition
IO	Inner- Outer method
STR	Stirred tank reactor
LDA	Laser Doppler Anemometry
QUICK	Quadratic Upstream Interpolation Convection Kinetics

ABSTRACT

The optimal design of stirred tank reactors and the understanding of the mixing mechanism depend mainly on the accurate prediction of its hydrodynamic. Turbulence models, of which the most commonly used is the standard $k-\epsilon$ equations, have been found to be incapable of accurately computing the turbulent flow field in stirred tank reactors. It was found, for instance, that the turbulent flow parameters ($C_{\epsilon 1}, C_{\epsilon 2}, C_{\mu}$) for the standard $k-\epsilon$ model cannot be regarded as universal for all flows (Rodi, 1984).

There have been several attempts to find a suitable set of model parameters for stirred tank reactors. In view of this, the present study investigated the performance of the standard $k-\epsilon$ model to predict the flow field in stirred tank reactors. The parametric analysis presented herein involves variation of the parameters in the model and an estimation of the overall error values between the experimental data and the model predictions, which includes the mean velocities and the turbulent kinetic energy. The analysis also involves ascertaining the stability of the model via the moment convergence approach. In this way, an optimum range of parameters for predicting the flow field in stirred tank reactors has been identified. However, it is worth noting that not all combinations of the parameters within this range will satisfy the two constraints established in the present study. The present study established that Abuejela and Lilley's (1984) set of parameters for recirculating flows used by Ranade and Joshi (1989), is not suitable for stirred tank reactors, as it has resulted in poor numerical and moment convergence. The findings of the present study also suggested that all the parameters had a significant effect on the flow field, which contrasts with the findings of Nere et al (2001).

To examine the trend of results within the optimum range of parameters, four different impeller configurations ranging from radial to axial types were used in this study. The axial impellers were 30° , 45° , 60° pitched blade turbines while the radial impeller was Rushton turbine.

An in-depth analysis showed that the optimum range of parameters gave an accurate representation of the mean flow field, and that there was a significant improvement in their predicted values of the turbulent kinetic energy. The combination of model parameters $C_{\mu} = 0.065$, $C_{\epsilon 1} = 1.2$, $C_{\epsilon 2} = 1.8$ has been proposed for predicting the turbulent flow field in stirred

tank reactors. This combination was obtained through a minimization of the error between the predicted and experimental values. However, the turbulent kinetic energy was underestimated in all the agitated vessels investigated. This suggested that the model parameters might not be responsible for the discrepancy. The present investigation concluded that the standard $k-\epsilon$ model should be modified specifically for stirred tank reactors, taking into consideration the turbulent intensity and the anisotropic nature of the flow field, which the present standard $k-\epsilon$ model and its variants do not address.

The commercial grid generation package GAMBIT was used to create body fitted structured grid nodes, and simulations were carried out using FLUENT, which is a commercial Computational Fluid Dynamics software package.

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CHAPTER ONE

1 INTRODUCTION

In process industries, stirred tank reactors (STR) are used for different operations such as gas dispersion, homogenisation, solid suspension and chemical reactions. The main function of stirred vessels is to ensure necessary bulk blending, heat transfer, micro-mixing and inter-phase transport processes. These processes are greatly affected by the hydrodynamics of flow in the agitated vessels, which largely depends on the configurations of both the impeller and the tank. There are several designs of impellers used in stirred vessels, which exhibit different performance characteristics. The flow pattern generated ranges from radial to axial. The reactor shape is usually cylindrical with either a flat or a dished bottom and a number of baffles. Figure 1.1 shows the schematic diagram of a typical stirred tank reactor. In most of its application, the flow in the vessel is complex and highly turbulent.

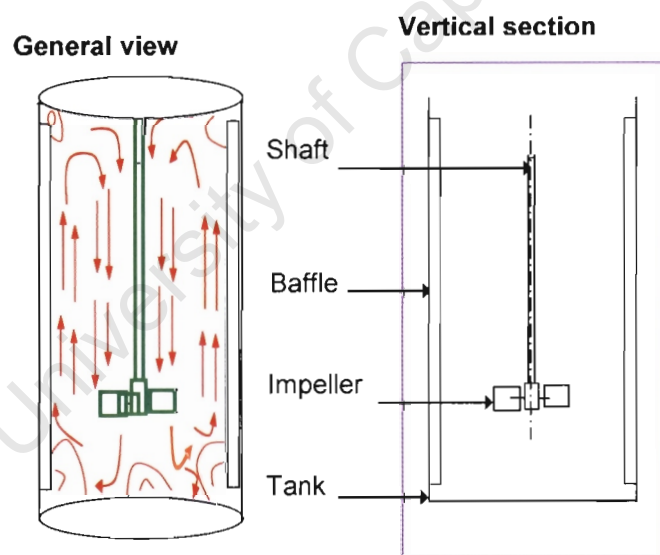


Figure 1:1: Schematic diagram of a Typical Stirred Tank Reactor

Despite the importance and wide applications of stirred tank reactors, their proper design and scale-up is uncertain. Smith (1989) reported that, in the United States, the lack of vital information about the mixing process resulted in improper plant design or modification and delay in process implementation, which accrued a loss of \$10 billion dollars annually. The new challenges also faced by these process industries are associated with increased market globalisation, demands for cleaner environments, higher customer expectations, drive for

increased profitability and the increasing demand to reduce time to market. These objectives can only be achieved through a detailed description of the flow field. This requires a better understanding of the hydrodynamics of flow in the STR so as to facilitate:

- Increase in the reaction yields
- Planned preventive and reactive maintenance
- Good product quality with no need for further purification, and
- Determination of key design objectives such as power consumption, mixing time and mass transfer coefficient

Several investigations (Ranade et al., 1990; Harris et al., 1996; Javed et al., 2006) have studied the hydrodynamics of flow in stirred tank reactor by means of experimental methods and numerical simulations, and are discussed below.

1.1 Experimental methods

Techniques such as pitot-tubes and hot wire anemometry have been used to measure the velocity fields in stirred tanks. The shortcoming of these techniques is their intrusive nature, which may affect the flow field measured. Advanced experimental methods such as Laser Doppler Anemometer (LDA) and Particle Image Velocimetry (PIV) were used to obtain detailed information about the flow field in stirred tank reactors (Ranade et al., 1989; Ashwin, 2001). The advantages of these techniques are their non-intrusive character and high resolution. However, these experimental studies have limitations regarding the scope of parameters that can be studied. For instance, the experimental methods require that the vessel and the operating liquid are translucent so as to ensure laser light transmission. In practice, though, most industrial stirred tank reactors are made of non-transparent materials and the operating liquids are opaque. In the case of gas-liquid flows too, the optical access to the flow becomes more difficult for higher gas fractions, which necessitates the use of small quantities to avoid light scattering in the LDA and bubble interference in PIV images (Deen, 2001). In addition, the non-intrusive character of the techniques makes them expensive and the operation necessitates specialised training (Ochieng, 2005). Due to the limitations in the experimental measurements and the fact that they may not be able to provide the comprehensive field data of the vessel, numerical simulation may be the best option.

1.2 Numerical Simulation

Computational Fluid Dynamics (CFD) involves the numerical solution of mass, momentum and energy in the flow system of interest, with additional sets of equations reflecting the actual situation. The incorporation of the CFD approach into the process industries has led to shortened product-process development cycles, optimization of existing processes, reduced energy requirements, efficient design of new products and processes, and reduced time to market. Its use has also facilitated the resolution of environmental, health and license to operate issues (Pordal et al., 2002). CFD has been identified as one of the technologies that will lead the chemical process industries into the future (The Chemical industry and the U.S Department of Energy, 1999). Studies have also shown that the CFD technique is an important and cost effective tool in the prediction and analysis of the flow field in the STR by providing a more detailed insight into the complex hydrodynamics (Ranade et al., 1989; Harris et al., 1996; Zhou et al., 2003).

1.3 Motivation and Aim

It is widely accepted that the Reynolds Averaged Navier Stokes Equations with an appropriate turbulence model will give a detailed description of the flow field (Jenne and Reuss, 1999). Raymond (2001) remarked that the computation of the turbulent flow field in agitated vessels is a challenge to the available turbulence models, of which the most commonly used is the standard $k-\varepsilon$ model. It is interesting to note that the standard $k-\varepsilon$ turbulence model gave the best results among the existing turbulence models and that using second moment closures did not improve the predictions of this flow field (Bakker et al., 1996; Monatee et al., 2001; Jaworski and Zakrzewska, 2002). Despite the good performance of the standard $k-\varepsilon$ model, the large discrepancy between the experimental data and the CFD values is yet to be resolved. Studies have remarked that the parameters (C_{ε_1} , C_{ε_2} , C_{μ}) for the standard $k-\varepsilon$ model were developed based on pipe flow and that it thus cannot be regarded as a general model (Rodi, 1984). It is further known that the flow field in a stirred tank reactor is completely different from that in a pipe flow. These parameters may thus need to be fine-tuned to achieve better predictions. There have been several attempts to do so, ranging from varying a single parameter at a time to zonal modelling but none of these approaches have fully addressed the disparity. In view of the above, a comprehensive parametric analysis is necessary to ascertain the possibility of a suitable set of model parameters for stirred tank reactors. There is also a need for a systematic approach to quantify

the errors between the experimental data and CFD values. This should give a better insight into the regions where high error values are expected. The current thesis will attempt to do this. In addition, the measured quantity that contributes predominantly to the global error will be determined.

1.4 Objective

The objective of this research is to carry out a detailed investigation of the performance of the standard $k - \epsilon$ model for stirred tank reactors considering its robustness, economy in terms of computing requirement and capability to predict industrial flows with high Reynolds number. Furthermore, how to quantify the errors obtained between predictions and experiments was investigated.

1.5 Structure of Thesis

The thesis is divided into five chapters:

- Chapter 1 provided the background and presented the aims and objective of this research.
- Chapter 2 presents the literature review on the governing transport equations for turbulent flows and the turbulence closure strategies. The numerical techniques and previous CFD studies on stirred tank reactors are also discussed.
- Chapter 3 sets out the CFD methodology and the parametric analysis procedures used in this study.
- Chapter 4 presents the results and discussion of the parametric analysis. It also shows the results for the mean velocities, turbulent kinetic energy for the standard $k - \epsilon$ model and the proposed optimum range. The performance of the optimum range of parameters in three different impeller stirred tank reactor configurations is discussed.
- In Chapter 5, the conclusions are drawn

CHAPTER TWO

2 LITERATURE REVIEW

An understanding of the hydrodynamics of flows is needed in many engineering problems. Fluid flow may be classified in various ways. The importance of each classification depends mainly on the particular application. These classifications include steady and unsteady, uniform and non-uniform, compressible and incompressible, laminar and turbulent types of flows. A flow is laminar when it is smooth and steady while turbulent flow is three-dimensional, unsteady, random, irregular, and rotational. These flows are governed by the conservation equations derived from mass, momentum, thermal energy and species concentration for a fluid element. For an incompressible flow, these equations are:

Continuity Equation:

$$\frac{\partial U_i}{\partial x_i} = 0 \quad 2.1$$

Momentum Equation:

$$\rho \frac{\partial U_i}{\partial t} + \rho U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \mu \frac{\partial^2 U_i}{\partial x_j \partial x_j} + \rho g_i \quad 2.2$$

Thermal energy/species concentration equation:

$$\frac{\partial \phi}{\partial t} + U_j \frac{\partial \phi}{\partial x_j} = \lambda \frac{\partial^2 \phi}{\partial x_j \partial x_j} + S_\phi \quad 2.3$$

where U_i is the velocity in the direction of x_j , P is the pressure, ρ is the density and ϕ is a scalar quantity, which may represent either temperature or species concentration. S_ϕ is a volumetric source term expressing, for instance heat generation due to chemical or biological reactions. μ and λ are the viscosity and diffusivity of ϕ respectively.

Most flows of engineering importance are turbulent in nature. It is broadly accepted that the numerical solution of Navier-Stokes equations together with the continuity equation provides a valid description of laminar and turbulent flows. This generates the pressure and velocity

fields in the flow domain. The established solution techniques for the Navier–Stokes equations are:

- Direct Numerical Simulation
- Large Eddy Simulation
- Turbulence Modelling

The Direct Numerical Simulation (DNS) approach entails solving the equations directly by using appropriate numerical procedures with suitable boundary conditions. This approach is not practicable in engineering applications due to the need to capture all eddies from the smallest scale, corresponding to dissipative motions, to the largest scale, corresponding to the largest dimension. In order to represent these fine scale turbulent eddies, the grid number required is about 2.25 times the power of the Reynolds number (Re) of the flow. For instance, in the case of a flow with Reynolds number 10^5 , which is often experienced in engineering applications, the number of grid nodes required would be higher than 10^{11} . Such a high number of required grid nodes would require large computational capacity, which would make the approach not feasible.

Large Eddy Simulation (LES) involves direct simulation of the three-dimensional, time-dependent large eddy structures, and it models small scale eddies smaller than the computational grid spacing. The application of LES to practical flows has been limited due to:

- Prohibitive computing cost at high Reynolds number
- The difficulties of specifying initial and boundary conditions and
- The need to perform three dimensional time dependent simulations, even if the flow is two dimensional and statistically stationary.

Both approaches (DNS and LES) are costly and time consuming in terms of computing requirements and are not practical in engineering applications. It is thus the third approach, Turbulence modelling, which was used in the current research.

2.1 Turbulence Modelling

In engineering design, the fine details of the turbulent motion are not needed, but rather its mean effect on the gross properties of the flow. Consequently, the turbulent flow fields can

be calculated with the Navier-Stokes system of equations averaged over space or time. When this averaging is performed, the equations describing the mean flow field contain the averages of products of fluctuating velocities. This additional term is referred to as Reynolds Stress, which results in more unknowns than the number of equations available. The process of determining or evaluating this additional term either by providing additional equations or solving it directly is referred to as **Turbulence modelling**. There are several ways of averaging the flow variables, which include time averages, ensemble averages, spatial averages and mass averages.

2.1.1 Time Averaging

This is mostly suitable for stationary turbulence in which the turbulent flow does not vary with time. For this type of flow, the instantaneous flow variable is expressed as $f(\mathbf{x}, t)$. The time averaging $F_T(\mathbf{x})$ is defined by

$$F_T(\mathbf{x}) = \frac{1}{\Delta t} \int_t^{t+\Delta t} f(\mathbf{x}, t) dt \quad 2.4$$

This approach is the most commonly used form of Reynolds averaging because turbulent flows are stationary in nature.

2.1.2 Ensemble Averaging

It is the most ideal type of Reynolds averaging when the flows decay with time. For instance, in terms of measurements of N identical experiments, $f(\mathbf{x}, t) = f_n(\mathbf{x}, t)$. The average (F_E) is defined as:

$$F_E(\mathbf{x}, t) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{n=1}^N f_n(\mathbf{x}, t) \quad 2.5$$

2.1.3 Spatial averaging

If the flow variable is uniform on the average such as in homogeneous turbulence, a volume integral can be used to do the averaging over all the spatial coordinates. This average (F_v) can be defined as:

$$F_v(\mathbf{x}, t) = \lim_{V \rightarrow \infty} \frac{1}{V} \iiint_V f(\mathbf{x}, t) \quad 2.6$$

2.1.4 Mass (Favre) Averaging

For compressible flows, it is often more expedient to use mass (Favre) averages instead of time averages

$$f = \tilde{f} + f'' \quad 2.7$$

where the mean quantity $\tilde{f}$ is defined as

$$\tilde{f} = \frac{\overline{\rho f}}{\rho} = \tilde{f} + \frac{\overline{p' f'}}{p} \quad 2.8$$

and the fluctuation f'' has the property

$$\overline{\rho f''} = 0 \quad 2.9$$

whereas $\overline{f''} = -\overline{p' f'}/\bar{p} \neq 0$

For incompressible flows, which are relevant in the present study, performing the time averaging on equations 2.1, 2.2 and 2.3 has resulted in the Reynolds Averaged Navier-Stokes (RANS) and Energy/Species Concentration equations as follows:

Continuity Equation

$$\frac{\partial U_i}{\partial X_i} = 0 \quad 2.10$$

Momentum Equation:

$$\rho \frac{\partial U_i}{\partial t} + \rho U_j \frac{\partial U_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \rho \frac{\partial}{\partial x_j} \left(\mu \frac{\partial U_i}{\partial x_j} - \overline{u_i u_j} \right) + \rho g_i \quad 2.11$$

Thermal Energy/Species Concentration Equation:

$$\frac{\partial \phi}{\partial t} + U_j \frac{\partial \phi}{\partial x_j} = \frac{\partial}{\partial x_i} \left(\lambda \frac{\partial \phi}{\partial x_i} - \overline{u_i \phi} \right) + S_\phi \quad 2.12$$

The terms $\overline{(\rho u_i u_j)}$ and $\overline{u_i \phi}$ in the momentum and energy/species concentration equations are referred to as Reynolds stress and scalar flux respectively. These Reynolds stress tensors

and Reynolds heat flux are the additional unknown variables that must be solved through turbulence modelling.

2.2 Turbulence Models

The different types of turbulence models can be broadly categorised as Eddy-viscosity models or Reynolds Stress models. The turbulence models that use the eddy-viscosity concept to determine the Reynolds stresses include:

- Zero Equation models
- One Equation models
- Two Equations models
 - Standard $k - \varepsilon$ model
 - RNG $k - \varepsilon$ model
 - $k - \omega$ model

The Eddy-viscosity concept is based on the assumption that turbulence is isotropic, and expresses the Reynolds Stress term as:

$$(\overline{\rho u_i u_j}) = \mu_t \left(\frac{\partial \overline{U_i}}{\partial X_j} + \frac{\partial \overline{U_j}}{\partial X_i} \right) - (2/3) \delta_{ij} k \quad 2.13$$

Where k is the turbulent kinetic energy and μ_t is the eddy viscosity that depends on turbulence and must be determined by the above stated turbulence models.

2.2.1 Zero Equation

The Zero-equation models close the system without providing additional differential equations. This can be achieved by the conventional method of Prandtl's mixing length model (Prandtl 1925). The recent zero equation models are Cebeci and Smith (1974) or Baldwin and Lomax (1978).

2.2.1.1 Prandtl's Mixing Length Model

Dimensional analysis indicates that dynamic turbulent viscosity is a function of fluid density (ρ), turbulent velocity scale (ϑ) and length scale (ℓ) as stated below:

$$\mu_t = C \rho \vartheta \ell \quad 2.14$$

where C is a dimensionless constant of proportionality.

Since most of the kinetic energy of turbulence is contained in the largest eddies, the turbulence length scale is therefore characteristic of these eddies, which interact with the mean flow.

The eddy length scale is represented as

$$\ell = c \ell \left| \frac{\partial U}{\partial y} \right| \quad 2.15$$

Combining equations (2.14) & (2.15)

$$\mu_t = \rho \ell_m^2 \left| \frac{\partial U}{\partial y} \right| \quad 2.16$$

where the ℓ_m Prandtl mixing length is given by $\ell_m = \kappa y$ with κ being the von Karman constant ($\kappa = 0.41$).

Equation 2.16 is referred to as Prandtl's mixing model. It is simple and computationally economical. It has been found to be suitable for simple shear layer dominated or pressure driven flows but unsuitable for complex flows. This is due to its inability to estimate the distribution of the mixing length and the transport effects of turbulence

All the proposed zero equation models fail to perform well in regions of recirculation or in separated flows (Wilcox, 2000).

2.2.2 One Equation Models

The eddy viscosity in the one-equation model approach is specified as

$$\mu_t = C_\mu \ell \sqrt{k} \quad 2.17$$

$$C_\mu = 0.09$$

where k is the turbulent kinetic energy

$$k = \frac{1}{2} \overline{U'_i U'_i} \quad 2.18$$

This process has introduced another variable k , in which a new governing equation must be given. The transport equation for this k is expressed as:

$$\frac{Dk}{Dt} = \frac{\partial}{\partial X_i} \left[\left(C_k \frac{k^2}{\varepsilon} + \nu \right) \frac{\partial k}{\partial X_i} \right] - \overline{u_i u_i} \frac{\partial U_i}{\partial X_i} - \varepsilon \quad 2.19$$

The performance of this model is not satisfactory and its predictability decreases when the flows are complex.

2.2.3 Two Equations models

There are several two-equation models, which will be discussed below. The eddy viscosity used in these models is expressed as:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \quad 2.20$$

The eddy viscosity contains two unknown variables k and ε referred as turbulent kinetic energy and turbulent kinetic energy dissipation rate respectively.

The turbulent kinetic energy dissipation rate is defined by this correlation as:

$$\varepsilon = \nu \overline{\frac{\partial u'_i}{\partial x_k} \frac{\partial u'_i}{\partial x_k}} \quad 2.21$$

The transport equation for the turbulent kinetic energy is derived by taking the time average of the product of the fluctuation component of the velocity with the turbulent flow momentum equations. After some algebra, the equations results in:

$$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = \tau_{ij} \frac{\partial U_i}{\partial x_j} - \varepsilon + \frac{\partial}{\partial x_j} \left(\nu \frac{\partial k}{\partial x_j} - \frac{1}{2} \overline{u'_i u'_i u'_j} - \frac{1}{\rho} \overline{p' u'_j} \right) \quad 2.22$$

The first and second terms on the right hand side of equation 2.22 is referred to as Production and dissipation respectively. The term with $\nu \partial k / \partial x_j$ is known as molecular diffusion and the

term with triple velocity correlation as turbulent diffusion. The last term on the right-hand side is known as pressure diffusion.

In a similar manner, the transport equation for ε can be derived by taking the time average of the product of $2\nu v'_{i,j}$, with the derivative of momentum equations.

$$\frac{\partial \varepsilon}{\partial t} + \frac{\partial \varepsilon}{\partial x_j} = A_{(\varepsilon)} + B_{(\varepsilon)} + C_{(\varepsilon)} \quad 2.23$$

with

$$\begin{aligned} A_{(\varepsilon)} &= 2\nu \left(\overline{u'_{i,k} u'_{j,k}} + \overline{u'_{k,i} u'_{k,j}} \right) \frac{\partial U_i}{\partial x_j} \\ B_{(\varepsilon)} &= -2\nu \overline{u'_k u'_{i,j}} \frac{\partial^2 U_i}{\partial x_k \partial x_j} - 2\nu \overline{u'_{i,k} u'_{i,m} u'_{k,m}} - 2\nu^2 \overline{u'_{i,k} u'_{k,m}} \\ C_{(\varepsilon)} &= \frac{\partial}{\partial x_j} \left(\nu \frac{\partial \varepsilon}{\partial x_j} - \nu \overline{u'_j u'_{i,m} u'_{i,m}} - 2 \frac{\nu}{\rho} \overline{p'_{,m} u'_{j,m}} \right) \end{aligned}$$

$A_{(\varepsilon)}$, $B_{(\varepsilon)}$, $C_{(\varepsilon)}$ represent the production, dissipation and transport terms respectively. The first, second and third terms in $C_{(\varepsilon)}$ are known as molecular dissipation, turbulent dissipation and pressure dissipation respectively.

As a result of more unknowns and the complexity of equation 2.23, Launder and Spalding (1974) proposed transport equations for k and ε to avoid such additional unknowns. This is referred as the standard $k - \varepsilon$ model.

2.2.3.1 Standard $k - \varepsilon$ Model

The transport equations for turbulent kinetic energy and its dissipation rate are solved so as to compute the turbulent viscosity for Reynolds Averaged Navier-Stokes (RANS) equations. Launder and Spalding (1974) proposed two equations for k and ε . These equations are referred to as the **Standard $k - \varepsilon$ model**.

$$\rho_i \frac{\partial k}{\partial x_i} = \mu_t \left(\frac{\partial \bar{u}_j}{\partial x_i} + \frac{\partial \bar{u}_i}{\partial x_j} \right) \frac{\partial \bar{u}_j}{\partial x_i} + \frac{\partial}{\partial x_i} \left[\left(\frac{\mu}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] - \rho \epsilon \quad 2.24$$

$$\rho \frac{\partial \epsilon}{\partial x_i} = C_{\epsilon 1} \frac{\epsilon}{k} \mu_t \left(\frac{\partial \bar{u}_j}{\partial x_i} + \frac{\partial \bar{u}_i}{\partial x_j} \right) \frac{\partial \bar{u}_j}{\partial x_i} + \frac{\partial}{\partial x_i} \left[\left(\frac{\mu}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_i} \right] - C_{\epsilon 2} \rho \frac{\epsilon^2}{k} \quad 2.25$$

$$C_{\epsilon 1} = 1.44, \quad C_{\epsilon 2} = 1.92, \quad C_\mu = 0.09, \quad \sigma_k = 1.0, \quad \sigma_\epsilon = 1.3$$

This model performs excellently for many flows of industrial importance. Consequently, it is the most commonly used turbulence model in the prediction of flows in stirred tank reactors. However, studies have shown that there are problems with the model in some unconfined flows and highly swirling flows because it does not contain a description of the subtle effects of streamline curvature (Versteeg and Malalasekera, 1995)

2.2.3.2 RNG k – ε Model

Due to the inadequacies of standard k – ε model that it does not give an accurate prediction in streamline curvature and near wall flow, a k – ε model was developed based on Renormalization theory Group techniques (Yakhot et al., 1992). This is stated below as expressed by Raymond et al. (2002):

$$\frac{Dk}{Dt} = \tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j} - \epsilon + \frac{\partial}{\partial x_j} \left[(\sigma_k \mu_{\text{eff}}) \frac{\partial k}{\partial x_j} \right] \quad 2.26$$

$$\frac{D\epsilon}{Dt} = C_{\epsilon 1} \frac{\epsilon}{k} \tau_{ij} \frac{\partial \bar{u}_i}{\partial x_j} - C_{\epsilon 2} \frac{\partial}{\partial x_j} \left[(\sigma_\epsilon \mu_{\text{eff}}) \frac{\partial \epsilon}{\partial x_j} \right] - R \quad 2.27$$

$$\text{where } R = \frac{C_\mu \eta^3 \left(1 - \frac{\eta}{\eta_0} \right) \epsilon^2}{1 + \beta \eta^3} \frac{1}{k}$$

$C_{\epsilon 1} = 1.44, \quad C_{\epsilon 2} = 1.68, \quad \eta = Sk/\epsilon, \quad \eta_0 = 4.38, \quad \beta = 0.012, \quad \sigma_\epsilon = 1.393 \quad \sigma_k = 1.393$
where S is the modulus of the mean rate of strain tensor.

2.2.3.3 k – ω Model

In this model, the turbulence associated vorticity ω is proportional to k^2/ℓ

$$\omega = c \frac{k^2}{\ell} \quad 2.28$$

Kinematic Eddy viscosity is

$$\nu_T = k/\omega \quad 2.29$$

The transport equations for k and ω as proposed by Wilcox (1998) are written as:

$$\frac{\partial k}{\partial t} + U_j \frac{\partial k}{\partial x_j} = \tau_{ij} \frac{\partial U_i}{\partial x_j} - \beta^* k \omega + \frac{\partial}{\partial x_j} \left[(\nu + \sigma^* \nu_T) \frac{\partial k}{\partial x_j} \right] \quad 2.30$$

$$\frac{\partial \omega}{\partial t} + U_j \frac{\partial \omega}{\partial x_j} = \alpha \frac{\omega}{k} \tau_{ij} \frac{\partial U_i}{\partial x_j} - \beta \omega^2 + \frac{\partial}{\partial x_j} \left[(\nu + \sigma^* \nu_T) \frac{\partial \omega}{\partial x_j} \right] \quad 2.31$$

with the closure constants

$$\alpha = 13/25, \beta = 3/40, \beta^* = 9/100, \sigma = 1/2, \sigma^* = 1/2$$

2.2.4 Reynolds Stress Models

The Reynolds stress models directly determine the unknown terms from the solution of differential transport equations in which they are the dependent variables. They accurately estimate the mean flow properties and all Reynolds stresses for many simple and complex flows, including wall jets, asymmetric, channel and non-circular duct flows and curved flows (Lauder et al., 1975; Jones and Musonge, 1988). The use of this model is limited due to the large computing requirements, and it has not been as widely validated as the $k-\varepsilon$ models (Aubin et al., 2004). Detailed explanation of the model is beyond the scope of this study.

2.2.5 Algebraic Stress Models

This model accounts for the anisotropy of Reynolds stresses economically without solving the complete set of Reynolds stress transport equations. It is not as widely validated as the $k-\varepsilon$ models and it is restricted to flows where the convection and diffusion terms are negligible (Versteeg and Malalasekera, 1995).

2.3 Treatment of Wall Bounded Flow

Proper representation of the influence of walls on turbulent flows is a significant feature in simulating wall-bounded flows, such as stirred tank reactors. At the wall boundary, there is a high velocity gradient and it requires excessive mesh refinements. In order to avoid such excessive mesh refinements, there are two main approaches to model the near-wall region. The first approach is the wall function; in this case, the viscosity-affected inner regions are

not modelled. The semi-empirical formula known as the wall function is used instead to link the viscosity-affected region between the wall and the turbulent region. This approach yields reasonable results without excessive computing requirements and is useful for modelling turbulent flows in stirred tank reactors. The second approach involves using low Reynolds number turbulence models to simulate the near wall region flow. This approach is not relevant to the present study and it will not be discussed.

In the wall functions approach proposed by Launder and Spalding (1974), a mean velocity profile is assumed to exist near the wall as shown:

$$u^+ = \frac{1}{\kappa} \ln y^+ + B \quad 2.32$$

where κ is the van Karmann constant (0.41), B is an empirical constant related to the thickness of the viscous sub-layer, y^+ is the dimensionless distance from the wall, and u^+ and y^+ are expressed as follows:

$$u^+ = \frac{U_t}{\sqrt{\tau_w / \rho}} \quad 2.33$$

$$y^+ = \frac{\rho n_p \sqrt{\tau_w / \rho}}{\mu} \quad 2.34$$

where n_p is the normal distance of the considered node at point P from the wall.

The flow is also assumed to be in local equilibrium; in other words, it is assumed that the production and dissipation terms are almost equal. This allows the use of a coarse mesh at the wall. The dimensionless distance of the adjacent grid node from the wall should be greater than 30 ($y^+ > 30$). The wall shear stress (τ_w) is then related to the tangential component of the velocity at the grid, and it is specified as:

$$\tau_w = \frac{\kappa \rho C_\mu^{1/4} \sqrt{k U_t}}{\ln(y^+ E)} \quad 2.35$$

For turbulent kinetic energy in the near-wall region, the normal gradient at the wall is set to zero. However, by assuming what the local equilibrium is, the turbulent energy dissipation

rate in the near wall region can be computed from an empirical relation as follows without solving the transport equation for ε :

$$\varepsilon = \frac{C_{\mu}^{3/4} k_P^{3/2}}{\kappa n_p} \quad 2.36$$

It should be noted that wall function is valid only when the first grid point is adjacent to the wall within the logarithmic region.

2.4 Numerical Techniques: Finite Volume Method

The governing transport equations of flow processes are non-linear and coupled partial differential, which can be solved numerically. The governing equations of complex flow system are mixed properties of hyperbolic, parabolic and elliptic. The parabolic equations describe time dependent problems with dissipative nature while the solution of hyperbolic equations contain discontinuities due to the non-dissipative nature of these equations. In the elliptic equations, the information propagates in all direction simultaneously and the solution is smooth. The sensitivity of parameters in non-linear partial differential equations cannot be underestimated. Consequently, these parameters greatly affect the model development, optimization, estimation and computational efficiency. The effects can be determined via the convergence, consistency and stability of the solution. A good understanding of the numerical solution algorithm is very important. The numerical solution of these equations replaces the continuous information contained in the exact solution of partial differential equations by discrete information available at a finite number of computational cells. The numerical method provides a set of discretized equations for these unknowns and prescribes an algorithm to solve these discretized equations. For any given differential equation, there are different methods to derive the discretized equations. These methods include finite element, finite difference and finite volume. In fluid mechanics, the finite element is primarily used for laminar flows, while the other methods are used for both laminar flows and turbulent flows. The finite volume method has been used in this study and it entails spatially integrating the governing transport equations over a finite control volume to obtain the set of discretized equations

2.4.1 Discretization of the Domain

The first step of the finite volume method is to divide the solution domain into a finite number of control volumes or computational cells. There are mainly two types of grids, namely structured and unstructured grids. In structured grid arrangements, there is a regular structure or topology, where the points of the mesh can be imagined as a grid of points placed in a regular way throughout a specific geometry as shown in Figure 2.1. The cells are hexahedral in nature and the position of a grid point is uniquely identified by a set of two or three indices in two or three-dimensional geometry respectively. The unstructured grids are irregularly structured in nature, which places no restrictions on the shape of the control volume and the number of neighbouring nodes. The cells are triangles and quadrilaterals in two-dimensional geometry, while they are tetrahedral or hexahedral in three-dimensional geometry, as shown in Figure 2.2. When a structured grid is used, there is an advantage in that the solver program should run faster than if the grid is unstructured. This is due to the implicit relationship that exists between the number of a cell or a point and the number of its neighbours in a structured mesh, which enables data to be found easily.

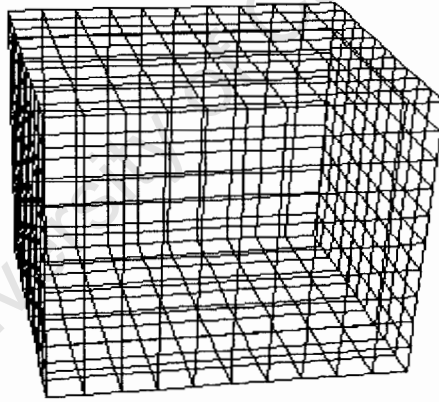


Figure 2:1: The structured grids arrangement

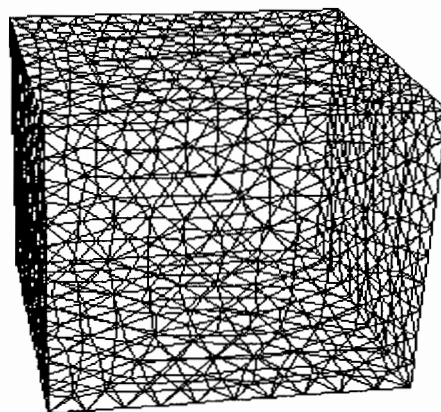


Figure 2:2: The unstructured grids arrangement

2.4.2 Discretization of Governing Transport Equations

The second step of the finite volume method is the discretization of the equations, which involves the integration of the governing transport equation over each computational cell or control volume and over the considered time interval Δt :

$$\int_t^{t+\Delta t} \left\{ \int_V \frac{\partial(\rho\phi)}{\partial t} dV + \int_S \rho U \phi \cdot n dS = \int_S \Gamma_\phi \nabla_\phi \cdot n dS + \int_V S_\phi dV \right\} dt \quad 2.37$$

where integration over V and S denotes volume and surface of a computational cell respectively, ϕ represents the dependent flow variable (u , v , w , k or ϵ), S_ϕ is the source term and Γ_ϕ is the diffusion coefficient

The integrated form of the equation contains unknown values of the dependent variable and its normal gradients at control volume faces. A detailed description of the integration steps can be found in Versteeg and Malasekara (1995). The behaviour of the finite volume method depends on the source term linearization employed and on the interpolation or discretization scheme. In order to have a solution that is numerically realistic, the discretization schemes must possess important properties like conservativeness, boundedness and transportiveness. In ensuring the overall conservation of ϕ , the flux of ϕ leaving a control volume across a given face must be equal to the flux of ϕ entering the adjacent control volume through the same face. Any numerical solution must be bounded by minimum and maximum boundary values if there is no source. The important requirement of boundedness is that all the coefficient of the discretized equation must be of the same sign and usually positive. The criterion of transportiveness can be illustrated by considering the distribution of ϕ in the vicinity of its source. The non-dimensional cell Peclet number (Pe) is measured by the ratio of strengths of convection and diffusion

$$Pe = \frac{F}{D} = \frac{\rho u}{\Gamma_\phi / \delta x} \quad 2.38$$

where δx is cell size, u is velocity, ρ is density and Γ_ϕ is the diffusion coefficient.

Some commonly used discretization schemes are central differencing, upwind, power-law, hybrid and Quadratic Upstream Interpolation for Convective Kinetics (QUICK). These are discussed briefly in the next paragraph.

In central differencing, the quantities are assumed to vary linearly between the two nearest nodal positions. To calculate the values at the control volume faces, a linear approximation is carried out. The accuracy of the central differencing scheme is second order, and the scheme will only be stable and accurate if $Pe < 2$. The limitation of central differencing is the inability to identify the flow direction and this makes it an unsuitable discretization scheme for general-purpose flow calculations. To address the transportiveness property, several discretization schemes have been proposed. The simplest is the first order upwind discretization scheme, which uses the nodal values to calculate the cell face values. This scheme is based on the backward differencing formula so the accuracy of this scheme is first order and is numerically diffusive. This numerical diffusion is increased in a multidimensional problem when the flow is not aligned with the grid but it can be addressed by refinement of the grid, although this is highly expensive.

In order to utilize the higher accuracy of the central differencing scheme, different combinations of central differencing and first order upwind discretization schemes were proposed. These include the hybrid differencing scheme (Spalding, 1972) and the power-law (Patankar, 1980). The principle of the hybrid differencing scheme is that the central differencing is used for small Peclet numbers ($Pe < 2$), whereas the upwind scheme is employed for large Peclet numbers ($Pe \geq 2$). This scheme is widely used in CFD methods and proved to be useful for predicting practical flows (Versteeg and Malasekara, 1995). The accuracy is first order, which is a disadvantage. With regards to the power-law scheme, the diffusion term is set to zero when the cell Pe is greater than 10. But if $0 < Pe < 10$, the flux is calculated by using a polynomial expression. The accuracy is also first order, but the results are better than those of the hybrid differencing scheme.

Furthermore, to ensure higher order accuracy, QUICK scheme of Leonard (1979) can be employed as well. In terms of this scheme, the cell face values are obtained by a quadratic function passing through two bracketing nodes (on each side of the face) and a node on the upstream side. The accuracy is third order, but it is more computationally demanding than the other approaches.

2.4.3 Boundary Conditions

The importance of boundary conditions in a solution domain cannot be underestimated. It is necessary to specify the appropriate initial conditions and boundary conditions when solving the closed set of governing transport equations. In this section, the commonly used boundary conditions, ranging from inlet boundary condition to periodic boundary condition, are discussed.

The inlet boundary is the surface where the surrounding environment communicates with the solution domain of interest. The information of flow properties entering the solution domain is usually known and that becomes the inlet boundary conditions. It must be noted that in the modelling of most agitated vessels, the solution domain is restricted to the vessel and the flow within the feed pipe is not modelled. The outlet boundary is the point where the flow exits from the solution domain. The outlet boundary condition means that the gradients normal to the outlet boundary are zero for the flow properties, except for the pressure. At the impermeable wall boundaries, a 'no slip' boundary condition is specified. This condition assumes that the fluid velocity on the solid surface is the same as that on the wall.

Another boundary condition is symmetry, which implies that the fictitious boundaries can be employed if the process equipment is repetitious or if the flow processes are symmetrical. This condition reduces the size and extent of the solution domain. At times, the solution domain may be geometrically symmetrical, but the flow pattern or processes may not. If this occurs, the entire solution domain should be considered.

The periodic boundary condition is applicable when the solution domain or its flow pattern is cyclically repeating in nature. In other words, the periodic boundary conditions are used when the flows across two opposite planes in a computational model are identical. Consequently, this condition reduces the size of the solution domain and the computing requirement.

2.4.4 Solution Algorithms

The two important issues in the Reynolds Averaged Navier-Stokes equation are the non-linearity of the momentum and the pressure-velocity coupling. The non-linearity of the momentum has been discussed earlier. In this section, the pressure-velocity coupling will be described. The peculiarity of the momentum equations is the role played by pressure. The

pressure gradients appear in the source term of the momentum equations, but there is no equation to calculate this pressure. It is thus indirectly calculated from the continuity equation. The process of calculating this pressure should ensure that the velocity field satisfies the continuity equation. A special treatment is required to ensure this pressure-velocity coupling. These methods include the Semi-Implicit for Pressure Linked (SIMPLE) method, the SIMPLE-Consistent (SIMPLEC) method, the SIMPLE-Revised (SIMPLER) method and the Pressure Implicit with Splitting Operators (PISO) method. All of these can be used for steady flow but only PISO and SIMPLEC can be employed for both steady and unsteady flows.

A comprehensive account of the numerical techniques discussed above can be found in Versteeg and Malasekara (1995) or Chung (2002).

2.5 Previous CFD Studies on the Stirred Tank Reactors

2.5.1 Impeller Modelling

The hydrodynamics modelling of the stirred tank reactor depends mainly on how the impeller is modelled. These modelling approaches include the impeller boundary condition, sliding grid (Luo et al., 1993), multiple frame of reference (Luo et al., 1994), inner and outer method (Brucato et al., 1994) and snapshot method (Ranade et al., 2002).

The impeller boundary condition (IBC) method is the conventional approach where the impeller is not explicitly simulated but its effects are modelled by imposing appropriate empirically derived boundary conditions on the external flow. The main constraints of this approach are that it is dependent on experimental data and that the boundary conditions are for specific tank geometries (Ranade et al., 1989; Sahu et al., 1998; Brucato et al., 1998). In addition, extending this approach to multi-phase flows in stirred vessel is not realistic because it is not possible to obtain accurate experimental boundary conditions at the impeller region, and details of flow within the impeller blade are essential for mixing and multiphase flows (Ranade, 1997).

Luo et al. (1993) proposed the sliding grid (SG) approach, in which the flow domain is divided into two cylindrical, non-overlapping sub-domains, where each grid is a separate block; the outer one is fixed with baffles, while the inner one rotates with the impeller. At the

interface, the finite volume mesh will shear or slide so as to take into consideration the relative motion between the two sub-domains. This solves the time-dependent form of the governing transport equation in the two domains (Luo et al., 1993; Jaworski et al., 1997).

The multiple frame of reference (MFR) approach is similar to the sliding grid; its computational approach is also carried out in two domains. The first domain moves at the impeller speed and is used to compute the flow around the impeller in a steady state, while the second domain is stationary and is used to calculate the flow away from the impeller. The solutions from the two domains are connected locally at the interface via velocity transformations from the domains (Luo et al., 1994). Both the SG and the MFR approach are similar but the difference is that SG is conducted in a transient mode while, for MFR, a pseudo-steady state is assumed. The SG approach is more computationally demanding because the transient terms must be solved. Several investigations have established that there is a negligible difference in the solutions from the sliding grid and that of the multiple frame of reference (Aubin et al., 2004). Tabor et al. (1996), for instance, compared the predictions from the SM and the MRF techniques against experimental data for the flow generated by a Rushton turbine. Both the SM and MRF approaches gave qualitatively good results. It was found that the MRF gave the best quantitative comparison with experimental data when finer grids are used, and that the SM calculation over-predicted the mean velocities.

In the inner-outer method, the whole tank is also divided into two partially overlapping zones with the inner domain containing the impeller, while the outer domain corresponds to the remaining part of the tank. The simulation is carried out in the inner domain with arbitrary boundary conditions imposed on the outer surfaces of the inner domain. As a result of this, the first set of values for the velocity and the turbulence quantities at the boundary surface of the impeller can be obtained. These values are used as boundary conditions for the first simulation of flow in the outer domain, as done in impeller boundary condition (IBC) approach. The solution of the outer region is used to provide boundary condition for the inner region. The results of the second inner domain simulation are then used as impeller boundary conditions for the second outer domain simulation. This procedure is repeated until a suitable numerical convergence is achieved.

Brucato et al. (1998) compared the numerical simulation results of the flow field in baffled mixing tanks, based on three different types of modelling approaches i.e. impeller boundary

conditions (IBC), inner-outer (IO) and sliding grid (SG) with the standard $k-\epsilon$ model, solved with either the hybrid or QUICK discretization scheme. The authors showed that the results of IBC method are very sensitive to the imposed boundary conditions and that the good predictions rely on the availability and accuracy of the empirical data for a specific geometry. The IO gave a better prediction compared to IBC modelling approach but it is more computationally demanding. The SG method gave the best agreement with the experimental data for the mean flow field but it under-predicted the turbulent kinetic energy. The other two methods yielded satisfactory results while it required no empirical information. In a similar manner, Montante et al. (2001) reported that the predictions from IO and SG are similar in quantitative agreement with the experimental data. The study concluded that the discrepancy in the predictions and experimental data does not depend on the computational strategy, i.e. the impeller modelling technique.

Ranade and Dommeti (1996) proposed the computational snapshot approach, where the impeller blades are considered stationary at a specific position. Appropriate momentum source and sink terms are specified to account for the impeller rotation. The authors assumed that flow in the stirred tank reactor is fully developed, which means that the flow within the impeller blades does not vary with time. Simulations were carried out using different impeller positions to obtain ensemble-average results. The approach was further validated in capturing the effects of trailing vortices behind the blades of a 45° downflow pitched blade turbine and a six-blade Rushton turbine; the results were satisfactorily in agreement with experimental data (Ranade et al., 2002).

2.5.2 Discretization Schemes

Sahu et al. (1995) compared three different first-order numerical schemes. These include the upwind scheme, the power-law scheme and the hybrid upwind scheme. Their study concluded that the power-law scheme is the most robust and accurate. In another investigation, Brucato et al. (1998) commented that the solutions obtained using the QUICK discretization scheme was not completely different from the hybrid upwind scheme, except for the higher recirculation rates in the top and bottom of the tank. Monatee et al. (2001) reported that the solutions from the hybrid-upwind and QUICK discretization schemes are identical. The authors observed that the discretization schemes do not have any effect on the predictions. Aubin et al. (2004) investigated three numerical schemes: first order upwind,

hybrid and QUICK. They reported that the type of numerical scheme does not affect the predictions of the mean velocities. However, all three schemes under-estimated the LDA turbulent kinetic energy data, and the first order upwind significantly under-predicted the quantity. The investigators remarked that the choice of discretization scheme is an important factor in the simulation of turbulent flows in stirred tank reactors.

2.5.3 Computational Grid Size

The geometry of stirred tank reactors is complex in nature. As a result, the choice of grid is an important factor that cannot be underestimated. Although the complex geometry of stirred tank reactors demands that the grid is unstructured, it is advisable to make it as structured as possible. A structured grid allows the flow to align with the grid arrangement. The properties of the solution algorithm depend on the type of grid and the arrangement of variables on the grid. If the algorithm is designed for a structured grid, it cannot be used for an unstructured grid. A finer grid should be used in the regions where sharp gradients are expected to take place.

The sharp gradients of mean velocities and turbulence quantities (k and ε) exist mainly in the impeller stream region of the stirred tank reactor. Consequently, local grid refinements should be used to resolve the region. It is expected that grid refinement will improve the computational accuracy, but the computing requirements should also be taken into consideration. Preliminary runs should also be carried out to ensure that the results are independent of the grid sizes. However, studies have shown that the differences observed between the experimental data and the predictions may not in fact be resolved by finer grids (Ng et al., 1998; Montante et al., 2001). The grid sizes used in previous studies have been compiled and presented in Table 2.1

Table 2.1: Illustration of grid sizes and system specifications used in previous studies

Reference	Tank Geometry, T = H (m)	Impeller type	Solution Domain	Grid Size
Ranade et al., 1989	0.3	45 ⁰ pitched blade turbine	90 ⁰	Not specified
Luo et al., 1993	0.294	Rushton turbine	360 ⁰	151,500
Luo et al., 1994	0.294	Rushton turbine	180	151,500
Xu Y and McGrath G, 1996	0.305	45 ⁰ pitched blade turbine	90 ⁰	61,000
Sahu et al., 1998	0.3	45 ⁰ pitched blade turbine	90 ⁰	22,000
Baker et al. 1998	0.3	45 ⁰ pitched blade turbine	90 ⁰	49,000
Nere et al., 2001	0.3	45 ⁰ pitched blade turbine	90 ⁰	Not specified
Ranade et al., 2002	0.15	45 ⁰ pitched blade turbine	90 ⁰	269,667
Bujalski et al, 2002	0.22	Rushton turbine	360 ⁰	130,000
Aubin et al., 2004	0.19	45 ⁰ pitched blade turbine	360 ⁰	155,000
Hartmann et al., 2004	0.15	Rushton turbine	360 ⁰	228,096
Khopkar et al., 2004	0.19	Axial flow Mixel TT	360 ⁰	283,500
Javed et al., 2006	0.294	Rushton turbine	180 ⁰	112,480

2.5.4 Turbulence Models

Several investigations have shown that the accurate prediction of the flow field in the stirred tank reactor is a challenge for the existing turbulence models (Raymond et al., 2001). Ranade et al. (1989) adopted the new set of model constants ($C_\mu = 0.125$, $C_{\epsilon_1} = 1.44$, $C_{\epsilon_2} = 1.6$, $\sigma_\epsilon = 1.3$, $\sigma_k = 1$, $\kappa = 0.14$) for the standard $k - \epsilon$ model developed and optimised by Abuejla and Lilley (1984) for recirculating flows in a combustor geometry. This yielded a better prediction compared to the standard $k - \epsilon$ model. The authors found that these parameters could be optimised to minimise the overall error between the predictions and the experimental data. In contrast, Brucato et al. (1998) commented that the use of the modified constant adopted by Ranade et al. (1989) failed to improve on the predictions and the effects were uncertain. In addition, Rodi (1993) remarked that the parameters (C_{ϵ_1} , C_{ϵ_2} , C_μ) for the standard $k - \epsilon$ model were developed based on pipe flow and it cannot be regarded as a general model. These parameters were modified for axisymmetric jet flow and yielded better predictions. It is known that the flow field is completely different in the stirred tank reactor

from the pipe flow. These parameters may need to be modified to achieve better predictions. Based on this, Sahu et al. (1995) studied the effects of the model parameters on flow variables. Their study showed that an increase in C_μ caused a reduction in the predicted circulation below the impeller region. It was observed that a lower value of the parameter $C_{\epsilon 2}$ resulted in an increase in the predicted circulation below the impeller, and in a decrease in the overall prediction of turbulent kinetic energy and the dissipation rate. It was noted that the $C_{\epsilon 1}$ affected the flow characteristics exactly in an opposite way to that of $C_{\epsilon 2}$. The study concluded that the parameters ($C_{\epsilon 1}$, $C_{\epsilon 2}$, C_μ) should be modified to achieve a better prediction of turbulent flow in the stirred tank reactor.

Sahu et al. (1998) furthermore observed that the parametric sensitivity study of Sahu et al. (1995) had revealed the possibility of achieving better predictions by adopting a zonal modelling approach. In this approach, the flow domains were divided into sub-domains and the parameter values were selected for each sub-domain via trial and error. It resulted in better predictions in all the flow variables except the turbulent energy dissipation rate. They established that the predictions of flow variables in the entire tank could be improved further by changing the turbulent model parameters at different zones.

In line with Sahu et al. (1998), there was a parametric sensitivity study of ($C_{\epsilon 1}$, $C_{\epsilon 2}$, C_μ) by Nere et al. (2001) to establish a method for parameter selection. In their analysis, when varying one of the parameters, the other set of parameters were kept constant, as they were in the standard $k-\epsilon$ model. It was observed that the flow predictions were relatively insensitive to the variation of $C_{\epsilon 1}$ and $C_{\epsilon 2}$. For C_μ , none of the simulations was able to give a satisfactory comparison. These findings contrast the conclusions of Sahu et al. (1995) above. Nere et al.'s (2001) study further investigated the original formulation of C_μ , which

is $\left(\frac{-\overline{u'v'}}{k} \right)^2$. This formulation was based on the conditions of the equilibrium shear layer, and

the experimental measurement of k and $-\overline{u'v'}$ in two-dimensional equilibrium shear layer gave 0.3 for the ratio of $(-\overline{u'v'}/k)$. It led to the value of 0.09 being used in the standard $k-\epsilon$ model. The authors agreed that C_μ should be considered as a parameter while the other parameters ($C_{\epsilon 1}$ and $C_{\epsilon 2}$) in the standard $k-\epsilon$ model should remain constant. Simulations were carried out based on their findings, and a linear proportionate relationship was established between C_μ and (k^2/ϵ) . This led to a new constitutive equation for eddy viscosity

formulation (new $k-\varepsilon$ model). The new $k-\varepsilon$ model was implemented in an in-house code, which yields a better prediction for the flow characteristics compared to the standard $k-\varepsilon$ model and the modified $k-\varepsilon$ model (Ranade et al., 1989). However, Ochieng et al. (2003) carried out a study on the hydrodynamics of a reactor with and without a draft tube. The simulation results were compared with the predictions made by Nere et al. (2001) and the experimental data in three regions of the vessel. It revealed that both predictions are better in the impeller region, whereas the predictions are poor in the regions closer to the liquid surface, which was attributed to the inability to model the free surface. The authors mentioned that the predictions were improved when the parameter ($C_{\varepsilon 2}$) in the standard $k-\varepsilon$ model was set to a higher value.

In another study to show the effect of turbulence models on CFD results, four different turbulence models (standard $k-\varepsilon$, realizable $k-\varepsilon$, RNG $k-\varepsilon$ and Reynolds stress model) were used to carry out simulations (Jaworski and Zakrzewska, 2002). The standard $k-\varepsilon$ model gave the best prediction of the mean axial velocity as compared to the other models. The turbulent kinetic energy was under-predicted irrespective of which model was used, but the standard $k-\varepsilon$ model indicated the least deviations from the experimental values. This agreed with earlier findings that the use of more complex models like the Reynolds stress models is not the solution to the discrepancies (Jenne and Reuss, 1999; Montante et al., 2001). In an attempt to resolve the disparity between the experimental and predicted values, the effects of the blade and the baffle thickness, the bottom wall friction, the grid size and the choice of turbulence models (Standard $k-\varepsilon$ model, RNG $k-\varepsilon$ and Reynolds stress models) were investigated by Montante et al. (2001). This investigation, however, had little or no effect in addressing the discrepancy.

Furthermore, Jenne and Reuss (1999) mentioned that the standard $k-\varepsilon$ model and other $k-\varepsilon$ variants would not perform well without modification. They concluded that the assumption of spectral equilibrium in these $k-\varepsilon$ models could be responsible for the discrepancy in the predicted and experimental values. The assumption means that the production of the turbulent kinetic energy is almost equal to the energy dissipation rate. However, in the stirred tank reactor, the turbulence production is mainly at the impeller region, which causes size differences of eddies in the entire tank.

Aubin et al. (2004) reported on the influence of modelling approaches, choice of turbulence models and numerical scheme. Their investigation was limited to the standard $k-\varepsilon$ model and the RNG $k-\varepsilon$ model, due to the inability of the Reynolds stress model to give a converged solution. Their study showed that there is little or no effect on the predictions of the mean velocities and the turbulence quantities by the two $k-\varepsilon$ models. The authors concluded that the differences between the predicted and measured turbulence quantities in a single phase must be addressed before proceeding to complex multiphase flows.

2.5.5 Performance Indicators

Several studies have compared different CFD modelling approaches in a more global manner by predicting some key performance indicators, such as power dissipation (P_0), Power number (N_p), mixing time and mass transfer coefficient.

Power dissipation is calculated from the rotational speed of the impeller and the torque of the blade, i.e. the forces acting on the impeller surfaces. Power dissipation is used to compute the power number N_p , and it is expressed as:

$$N_p = \frac{P_0}{\rho N^3 D^5} \quad 2.39$$

where P_0 is the power dissipation, ρ is the density of the fluid, N is the impeller's rotational speed and D is the diameter of the impeller.

Brucato et al. (1998) reported on the sensitivity of the Power number to the impeller boundary conditions and also its sensitivity to different grid sizes when the inner-outer method is used. The authors found that the Power number value predicted by the sliding grid method is in best agreement with the experimental data. Ashwin (2001) compared the power number computed by three methods, which included volume integration of local ε values, the balance of forces acting on the impeller blades, and outflow angular momentum from the impeller zone. The study ascertained that the Power number obtained by means of the volume integration and forces balance techniques compared reasonably well with the experimental data, whereas the angular momentum concept slightly under-predicted the Power number. In comparing the effects of the different modelling approaches on power dissipation, Aubin et al. (2004) concluded that the power consumption values predicted by the sliding grid and

multiple frame reference are similar and in good agreement with the experimental data. The study also established that the type of discretization scheme has a noticeable effect on the predictions of power consumption, with the first-order upwind and QUICK schemes underpredicting. The two turbulence models (standard $k-\varepsilon$ and RNG $k-\varepsilon$) gave similar values for power consumption. Ochieng and Lewis (2004) evaluated the mean energy dissipation rate at different impeller clearances (0.33T and 0.15T). Their study concluded that lower homogenisation energy can be achieved with a lower clearance (0.15T) configuration. This was attributed to the higher Power number obtained at the higher impeller clearance (0.33T).

The simulation of mixing involves introducing a secondary liquid as an inert into the primary liquid in the vessel and then monitoring the tracer concentration as a function of time. Mixing time is defined as the time required for the tracer concentration to reach 95% of final concentration. The mixing process occurs due to the transport at three levels: molecular, eddy and bulk motion. Sahu et al. (1999) compared the mixing time for a pitched blade turbine in three different tank diameters and at various levels of power consumption. The predicted values deviated from experimental values by 5-10%. Zhou et al. (2003) reported that the mixing simulation depends largely on the flow field. This means that the accurate flow prediction provides a sound base for mixing simulations. Their study also revealed that the position of tracer addition and detecting position tend to give different mixing times, which is in agreement with earlier findings of Bujalski et al. (2002). Javed et al. (2006) carried out the simulation of mixing and its hydrodynamics and their study concluded that the predicted mixing time values deviated from the experimental values by 16%. The mean flow structure and level of turbulence in tank were found to have a significant effect on the spatial distribution of the tracer concentration.

In view of all the previous studies, there is clearly a need for a comprehensive parametric analysis of the standard $k-\varepsilon$ model to determine a suitable set of parameters for the prediction of the hydrodynamics of stirred tank reactors. The possibility of quantifying the discrepancy between the experimental data and the CFD values needs to be explored to enhance understanding of the model's performance. This is the basis for the approach used in the present study.

CHAPTER THREE

3 CFD METHODOLOGY

FLUENT, a commercial CFD software package developed by FLUENT, Inc was used in this study. It includes a mesh generation module called GAMBIT and a solver. The pre-processor GAMBIT is a comprehensive package for grid generation, and it is used to create a wide variety of structured and unstructured grids in two and three dimensions. The general modeling capabilities of FLUENT relevant to this study are:

- 3-D axisymmetric flows with swirl (rotationally symmetric)
- Finite volume method
- Choice of segregated and coupled solvers: In a segregated solver the governing equations are solved sequentially whereas in a coupled solver they are solved simultaneously.
- Steady state or transient analysis
- Incompressible flows
- Multiple reference frame (MFR) and sliding mesh options
- Turbulent flows and
- Extensive material property database.

The CFD analysis conducted in this study can be divided into three main steps (*pre-processing, solution and post processing*) as shown in Figure 3.1:

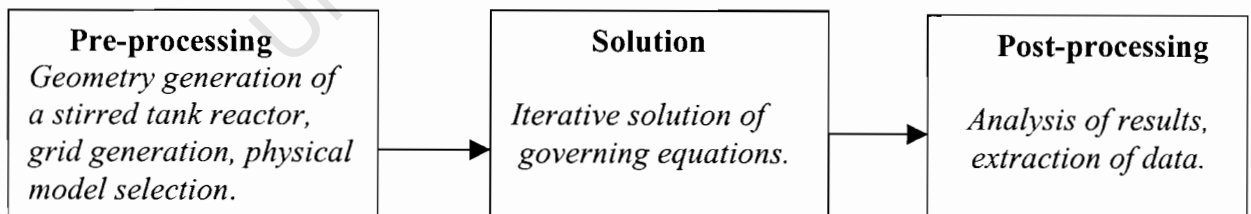


Figure 3.1: Flow charts for CFD analysis

Pre-processing involves the geometrical representation of a stirred tank reactor, defining a suitable mesh and applying the principles of flow physics. Mesh generation is a critical step in CFD analysis, where the governing equations are solved at discrete locations in the flow system. The accuracy of CFD analysis and the computing requirements depend primarily on

the mesh quality. After the pre-processing stage has been completed, the actual computation of the whole process entails the specification of a numerical discretization technique, and a solver is used to generate a solution. The governing equations are highly coupled and non-linear in nature. Consequently, a guess and correct iterative strategy is implemented to compute the solution. Information will be provided so as to obtain a stable converged solution. Lastly, in the post-processing step, the results are analysed to confirm if the solution is physically realistic. This will be accomplished by plotting the flow variables in a line or in a three-dimensional plane so as to give a representation of the flow field.

3.1 Vessel Geometry

The tank geometry employed for the parametric analysis was a flat-bottomed cylindrical tank of diameter $T = 0.3\text{m}$, with liquid height equal to the tank diameter ($H=T$) and four equally spaced vertical baffles of width $B = T/10$. A standard 45° pitched blade turbine with diameter $D = T/3$, hub diameter $d_h = 0.25D$, blade width, $w_b = 0.3D$, blade thickness of $0.02D$ was positioned at $C = T/3$. The rotational speed (N) for the impeller was 300rpm (5Hz), corresponding to a Reynolds number (Re) of 49760. In view of the need to predict the hydrodynamics accurately before looking at complex multiphase flows, a single phase was considered for the present investigation and the operating fluid was water with density (ρ) = 998.2kgm^{-3} and viscosity (μ) = 0.001003kg/m-s .

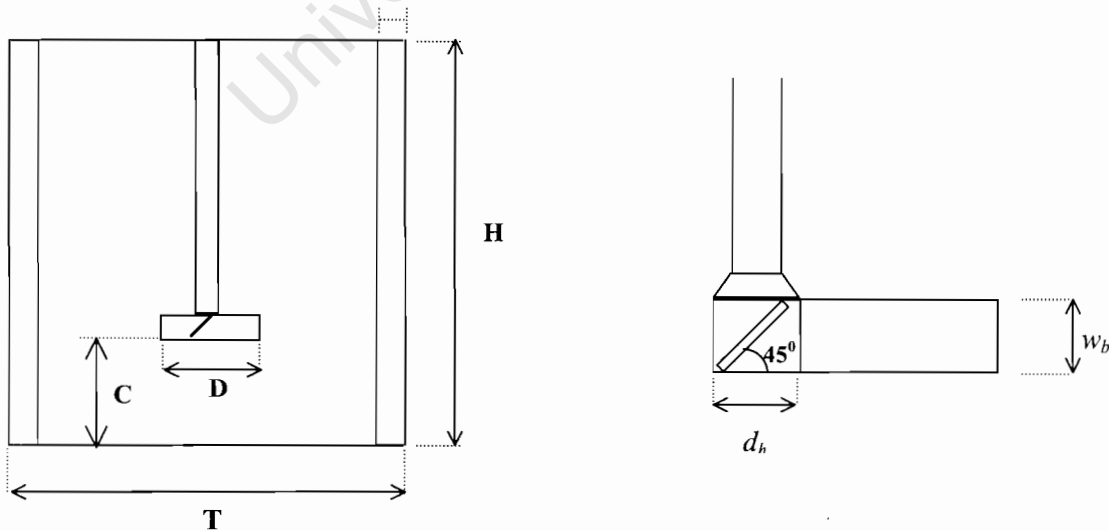


Figure 3:2: Schematic diagram of a baffled tank with 45° pitched blade turbine

Experimental studies have shown that the shape of the impellers and the blade angles have a significant influence on the flow field in stirred tank reactors (Ranade and Joshi, 1989; Chapple, 2002). To ascertain the adequacy of the proposed optimum set of parameters in predicting the flow characteristics of any impeller, three different geometries ranging from axial to radial flow impellers were modelled using structured grids. The geometries included the axial flow 30° pitched blade turbine and 60° pitched blade turbine stirred tank reactors used by Ashwin (2001), as well as the geometrical details of the Rushton turbine presented in Javed et al. (2006). The schematic diagram of a baffled tank with a Ruston turbine impeller that generates a radial flow pattern is shown in Figure 3.3. These geometries were selected from published literature based on the availability of comprehensive experimental data. The dimensions and other details of the vessels are illustrated in Table 3.1

Table 3.1: Geometrical details of the agitated tanks

Geometrical details	Tank 1	Tank 2	Tank 3
Tank diameter (T) (m)	0.5	0.5	0.296
Height (H)	T	T	T
Baffle (B)	T/10	T/10	T/10
Impeller type	60° pitched blade turbine (6 blades)	30° pitched blade turbine (6 blades)	Rushton turbine (6 blades)
Impeller diameter (D)	T/3	T/3	T/3
Impeller clearance (C)	T/3	T/3	T/3
Blade length (l_b)	-	-	D/4
Disc diameter (d)	-	-	0.75D
Hub diameter (d_h)	0.25D	0.25D	0.25D
Rotational speed of the impeller (N) (rpm)	160	160	300

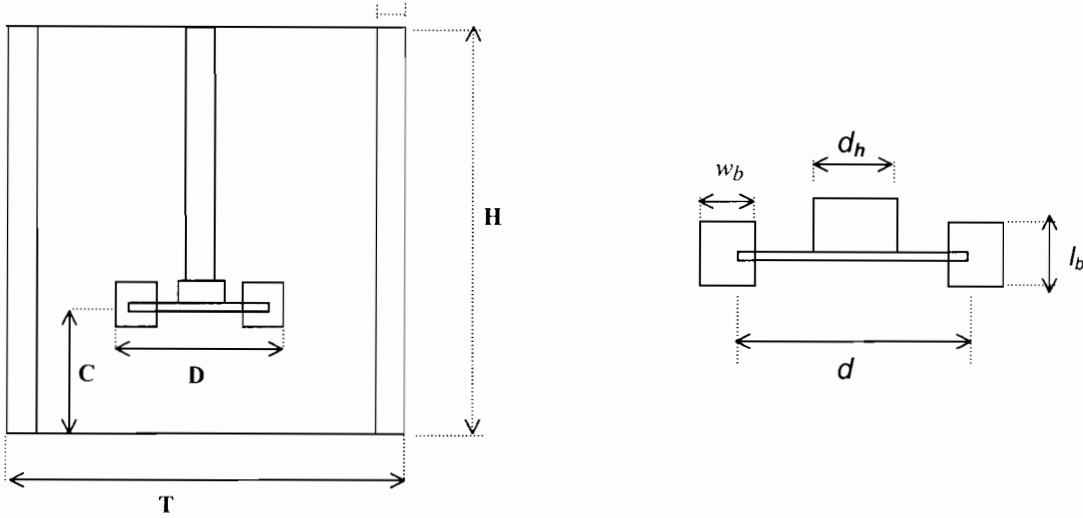


Figure 3:3 : Schematic diagram of a baffled tank with Ruston turbine impeller

3.2 Grid Generation

The commercial grid generation package GAMBIT (FLUENT Inc.) was used to create body fitted structured grid nodes for all the geometries studied. For 30° , 45° and 60° pitched blade turbines respectively, the whole tank was used in the simulation due to the overlapping nature of the blades relative to the diameter of the hub. Simulating the flow generated by the six bladed Rushton turbine, half of the tank comprising three impeller blades and two baffles was considered as solution domain by applying a periodic boundary condition on the symmetry plane as shown in Figure 3.4. Periodic boundary conditions were used when the flows across two opposite planes in a computational model were identical (Fluent 6.2). This reduced the computing requirement.

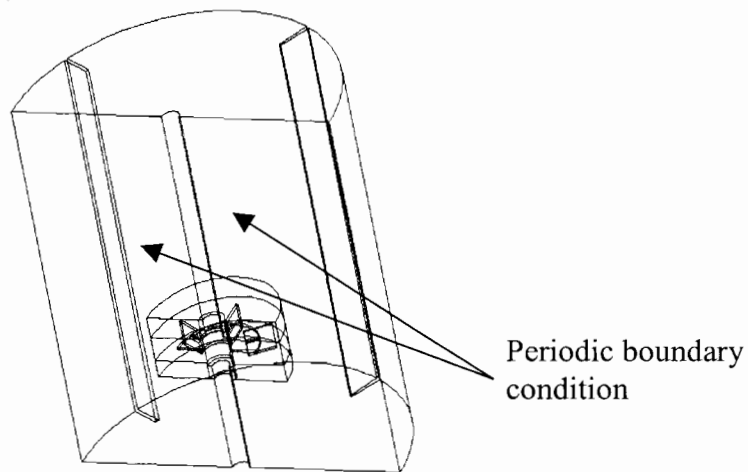


Figure 3:4: The periodic boundary condition

The multi block approach was adopted to construct the mesh by dividing the domain into a number of blocks due to the complex nature of the stirred tank reactor, especially around the impeller region. The topology of the overall grid was determined by the arrangement of the blocks, and a simple grid was generated in each block. The use of structured multi-block grids facilitates the generation of good quality grids for extremely complex geometries like stirred tank reactors, as shown in Figure 3.5. This approach also helps in refining the grid around the region of high velocity gradients. For example, in order to capture the trailing vortices, additional nodes were placed on the surface of the impeller blades as indicated in Figure 3.6.

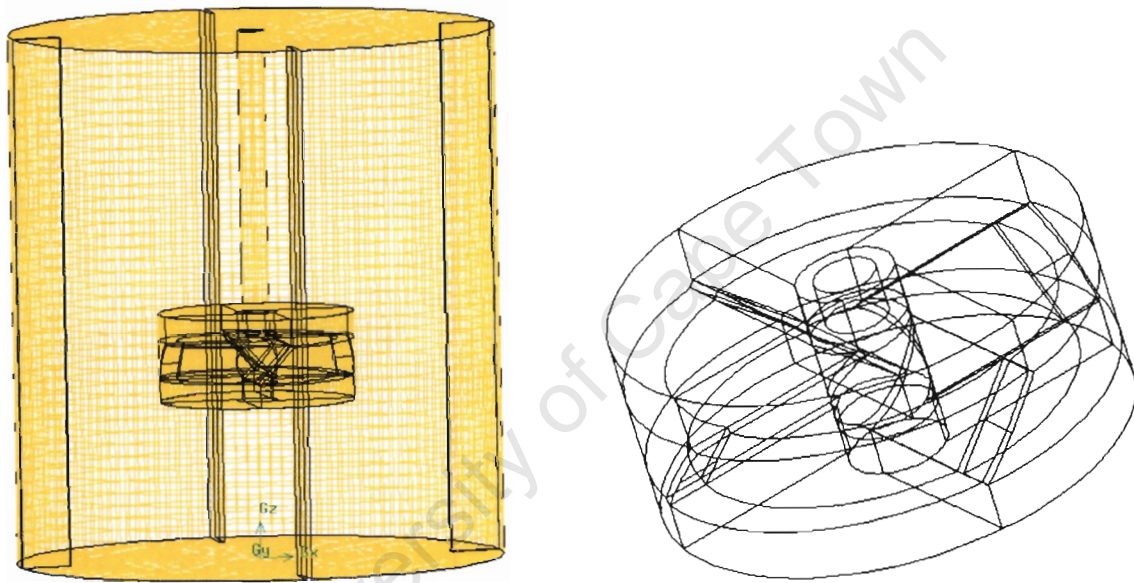


Figure 3:5: The multi-block arrangement in the tank and around the impeller region.

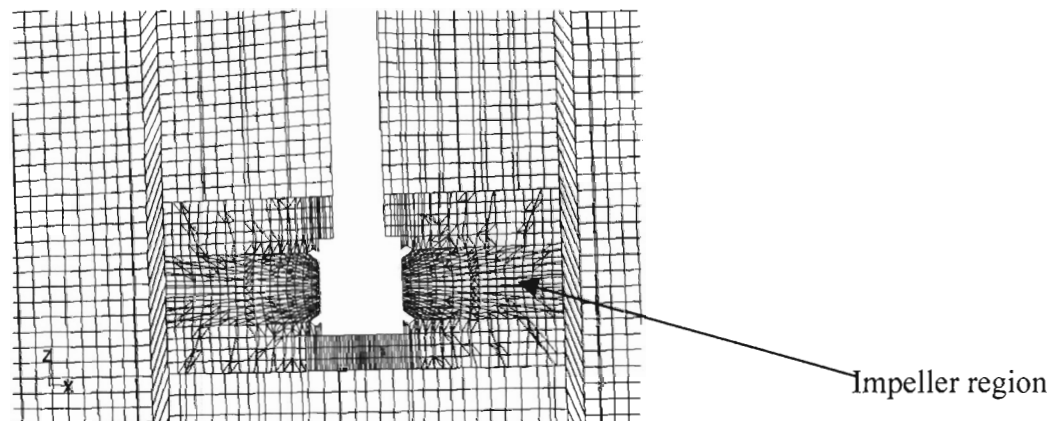


Figure 3:6: Cross- sectional area of the tank showing the grid refinement around the impeller region

Preliminary runs were carried out for all the geometries to ensure grid independence. This grid independence study was done to ascertain that the accuracy of the solution is indeed independent of grid size. The grid sizes for the different geometries are presented in Table 3.2. The solving of the Reynolds Averaged Navier-Stokes (RANS) equations and the turbulence equation was done on a Pentium 4, 2GB RAM, 3.20GHz PC. The average computing time was 12 hours for each run of simulation.

Table 3.2: Grid sizes for the different geometries

	GRID 1	GRID 2	GRID 3	GRID 4
45 ⁰ pitched blade turbine	88690	174000	282776	367628
30 ⁰ pitched blade turbine	184200	363994	527968	-
60 ⁰ pitched blade turbine	162344	340717	451094	507539
Rushton turbine	73500	91502	112522	135065

3.3 Boundary Conditions

The impeller blades and baffles were modelled as walls, and a 'no slip' boundary condition was specified for the vessel walls. The top surface of the liquid was modelled as a free surface with a zero shear stress condition. The interaction between the impeller and the baffles was modelled using the multiple frame of reference (MFR) approach (Luo et al., 1994). An angular velocity corresponding to the impeller rotational speed was specified for the impeller shaft, hub and disc in the case of the Rushton turbine. A cyclic boundary condition was imposed on the periodic planes of the Rushton turbine as shown in Figure 3.4.

3.4 Discretization Schemes

The Power Law, second upwind and QUICK discretization schemes were used in the preliminary studies to determine their effect on the predicted results. The most appropriate discretization scheme was determined and implemented in subsequent simulations.

3.5 Solution algorithm

The discretized Reynolds Averaged Navier-Stokes (RANS) equations were coupled with the pressure correction equation by adopting the Semi-Implicit Method for the Pressure Linked Equations (SIMPLE) algorithm. In this method, a guess pressure was used to solve the discretized momentum equations. The velocity values computed by solving these equations

did not satisfy the continuity equation, and corrections to these velocities were thus established. Based on the velocity corrections, a pressure correction was calculated, which was added to the original guessed pressure to give an updated pressure. The k and ϵ equations were solved using the corrected velocities. The entire process was repeated until a converged solution was achieved.

3.6 Convergence Criteria

The convergence criteria are preset conditions for the normalized or scaled residuals that determine when an iterative solution has converged. There is an assumption that the solution would no longer change when the convergence criteria have been attained, and this resulted in an overall mass balance throughout the domain. In the present analysis, the solution was considered to have converged when the total normalized residual for the continuity equation dropped below 1×10^{-4} .

3.7 Procedure for the Parametric Analysis

To achieve the aim of the study, the parameters were varied based on the 3^3 factorial design for each set of simulations. The design of each set resulted in 27 different combinations. The factorial design concept examines the interaction effects that exist between parameters. In addition, it facilitates the investigation of two or more parameters simultaneously, instead of conducting independent studies. The variation of the parameters was done within the range as indicated in Table 3.3 and this covered the scope of previous parametric studies. The entire parametric process entailed four different sets of simulations, which gave 104 different combinations. The various combinations of the parameters are illustrated in Tables 3.4, 3.5, 3.6 and 3.7.

Table 3.3: Range of parameters combination

Parameters	Range
C_μ	$0.01 - 0.18$
$C\epsilon_1$	$0.9 - 1.6$
$C\epsilon_2$	$1.4 - 2.8$

Table 3.4: Turbulence model parameters for the first set of simulations

C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$
0.05	0.9	2.8	0.115	0.9	2.8	0.18	0.9	2.8
0.05	0.9	2.1	0.115	0.9	2.1	0.18	0.9	2.1
0.05	0.9	1.4	0.115	0.9	1.4	0.18	0.9	1.4
0.05	1.25	2.8	0.115	1.25	2.8	0.18	1.25	2.8
0.05	1.25	2.1	0.115	1.25	2.1	0.18	1.25	2.1
0.05	1.25	1.4	0.115	1.25	1.4	0.18	1.25	1.4
0.05	1.6	2.8	0.115	1.6	2.8	0.18	1.6	2.8
0.05	1.6	2.1	0.115	1.6	2.1	0.18	1.6	2.1
0.05	1.6	1.4	0.115	1.6	1.4	0.18	1.6	1.4

Table 3.5: Turbulence model parameters for the second set of simulations

C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$
0.03	1	2.6	0.065	1	2.6	0.1	1	2.6
0.03	1	2.6	0.065	1	2.6	0.1	1	2.6
0.03	1	2.6	0.065	1	2.6	0.1	1	2.6
0.03	1.2	2.2	0.065	1.2	2.2	0.1	1.2	2.2
0.03	1.2	2.2	0.065	1.2	2.2	0.1	1.2	2.2
0.03	1.2	2.2	0.065	1.2	2.2	0.1	1.2	2.2
0.03	1.4	1.8	0.065	1.4	1.8	0.1	1.4	1.8
0.03	1.4	1.8	0.065	1.4	1.8	0.1	1.4	1.8
0.03	1.4	1.8	0.065	1.4	1.8	0.1	1.4	1.8

Table 3.6: Turbulence model parameters for the third set of simulations

C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$
0.045	1.1	2.4	0.07	1.1	2.4	0.095	1.1	2.4
0.045	1.1	2.2	0.07	1.1	2.2	0.095	1.1	2.2
0.045	1.1	2	0.07	1.1	2	0.095	1.1	2
0.045	1.25	2.4	0.07	1.25	2.4	0.095	1.25	2.4
0.045	1.25	2.2	0.07	1.25	2.2	0.095	1.25	2.2
0.045	1.25	2	0.07	1.25	2	0.095	1.25	2
0.045	1.4	2.4	0.07	1.4	2.4	0.095	1.4	2.4
0.045	1.4	2.2	0.07	1.4	2.2	0.095	1.4	2.2
0.045	1.4	2	0.07	1.4	2	0.095	1.4	2

Table 3.7: Turbulence model parameters for the fourth set of simulations

C_μ	$C_{\epsilon 1}$	$C_{\epsilon 2}$	C_μ	$C_{\epsilon 1}$	$C_{\epsilon 2}$	C_μ	$C_{\epsilon 1}$	$C_{\epsilon 2}$
0.045	1.22	2.15	0.0675	1.22	2.15	0.09	1.22	2.15
0.045	1.22	1.95	0.0675	1.22	1.95	0.09	1.22	1.95
0.045	1.22	1.75	0.0675	1.22	1.75	0.09	1.22	1.75
0.045	1.31	2.15	0.0675	1.31	2.15	0.09	1.31	2.15
0.045	1.31	1.95	0.0675	1.31	1.95	0.09	1.31	1.95
0.045	1.31	1.75	0.0675	1.31	1.75	0.09	1.31	1.75
0.045	1.39	2.15	0.0675	1.39	2.15	0.09	1.39	2.15
0.045	1.39	1.95	0.0675	1.39	1.95	0.09	1.39	1.95
0.045	1.39	1.75	0.0675	1.39	1.75	0.09	1.39	1.75

In view of the performance analysis and the need to establish a systematic approach in quantifying the discrepancies, two different criteria were identified to critically analyse the results:

- Error values of the CFD predictions and the experimental data
- Power number

These approaches were combined as tools to appraise the model results, and are discussed in the following sections.

3.7.1 Error Analysis

In engineering practice, an error is the difference between the actual value and the predicted value. There are two main types of errors: Fixed errors and random errors. Fixed errors are the ones that will cause repeated readings to be in error. They could also be termed systematic or bias errors. Random errors are caused by personal fluctuations, random electronic fluctuations in the instruments, or various influences of computation techniques. This type of error sometimes tends to follow a certain statistical distribution. As a result, there are different types of error estimation tools. To ensure consistency in the determination of the error values in the current research, the following two major tools for error analysis were used to determine the error values between the experimental data and the CFD predicted values:

- Standard error of the estimate
- The method of Least Squares.

3.7.1.1 Standard Error of the Estimate

The standard error of the estimate method is an evaluation of the accuracy of predictions carried out with a regression line. The regression line minimizes the sum of the squared errors of prediction. The process involves the difference between the experimental data and the predicted values. The difference is squared and the square root of the average squared error of prediction is used as a measure of the accuracy of prediction. This estimated value is referred to as the standard error of the estimate ($\sigma_{est.}$) and is expressed as:

$$\sigma_{est} = \sqrt{\frac{\sum (Y - Y')^2}{N}} \quad 3.1$$

Where Y is the experimental value, Y' is the predicted value, N is the number of point

3.7.1.2 Method of least squares

The underlying principle of this approach is that the best-fit line has the minimal sum of the deviations squared from a specified set of data. Suppose there is a sample of n data points (x_1, y_1), (x_2, y_2),..... (x_n, y_n) where x is the experimental value and y is the predicted value. It should be emphasised that the fundamental principle is that x is either free from error or subject to negligible error only, while y is subjected to errors, which can be eliminated with the method of least squares. The fitting line $f(x)$ has the deviation (d) from each data point, i.e. $d_1 = y_1 - f(x_1)$, $d_2 = y_2 - f(x_2)$,..., $d_n = y_n - f(x_n)$. According to the method of least squares, the best fitting line has the property that:

$$\Pi = d_1^2 + d_2^2 + \dots + d_n^2 = \sum_{i=1}^n d_i^2 = \sum_{i=1}^n [y_i - f(x_i)]^2 = \text{a minimum} \quad 3.2$$

3.7.2 Power number

The second criterion, the Power number (N_p), is a key design objective for stirred tank reactors. It was computed from the power dissipation calculated from the rotational speed of the impeller and the torque of the blade, i.e. the moment acting on the impeller surfaces. The torque on each blade can be calculated in FLUENT 6.2 as:

$$M = \underbrace{\vec{r}_{AB} \times \vec{F}_p}_{\text{pressure moment}} + \underbrace{\vec{r}_{AB} \times \vec{F}_V}_{\text{viscous moment}} \quad 3.3$$

where A represents the specified moment centre, B is the force origin $\vec{r}_{AB}$ is the moment vector, $\vec{F}_p$ is pressure force vector, and $\vec{F}_v$ is the viscous force vector.

Subsequently, the power required for rotation of the impeller at a steady rotational speed of N revolutions per second for an impeller is given by:

$$P_0 = 2\pi NM \quad 3.4$$

where N is the rotational speed in revolutions per second, and M is the torque

In calculating the torque of the blade, i.e. its moment, its convergence was monitored in the commercial CFD package FLUENT. Convergence was achieved once the moment attains a constant value over a number of iterations. If the moment does not converge, this is an indication that the model is not ideal for that particular situation or that the solution has not reached convergence. In this study, the parameters in the standard $k-\epsilon$ model were varied; the inability of some combinations to converge was an indication that the parameters were affecting the stability of the model. For instance, the default parameters in the standard $k-\epsilon$ model resulted in good moment convergence, but some of the parameter combinations did not. This poor convergence implied that the model was unsuitable for predicting flow field in stirred tank reactors.

The Power number is then expressed as:

$$N_p = \frac{P_0}{\rho N^3 D^5} \quad 3.5$$

where P_0 is the Power consumption, ρ is the density of the operating fluid, N is the rotational speed, and D is the impeller diameter.

CHAPTER 4

4 RESULTS AND DISCUSSION

The mean velocities and turbulent kinetic energy predictions for the 45⁰ pitched blade turbine were compared with the experimental Laser Doppler Anemometer (LDA) data presented in Sahu et al. (1998), and the geometry was used for the performance analysis as mentioned earlier (see section 3.1). The CFD predictions for the 30⁰ and 60⁰ pitched blade turbine were validated with the experimental data published in Ashwin (2000). For the Rushton turbine, the available (LDA) data in Javed et al. (2006) were used to validate the predictions. Studies have shown that the LDA measurement of the turbulent kinetic energy dissipation is uncertain and that the CFD predictions are also poor (Ng et al., 1998; Sahu et al., 1998). Consequently, these predictions were not validated in the present work. All the mean velocities and the turbulence kinetic energy were normalised with U_{tip} and U_{tip}^2 respectively, while the radial co-ordinates were normalised with the radius of the tank (R).

4.1 Discretization scheme

Preliminary simulations were carried out with three discretization schemes namely: Power-law, second order upwind, and QUICK to ascertain the effect on CFD predictions. It is expected that higher order discretization schemes will give more accurate results, but they are often less robust and more computationally demanding. The plots of the mean velocities and turbulent kinetic energy at the different levels of the tank are shown in Appendix A. The present study ascertained that the discretization schemes had little or no effect on the mean velocities. It was also established that the type of differencing scheme significantly influences the turbulent kinetic energy predictions. This agrees with the earlier findings of Aubin et al. (2004). The second order upwind and QUICK schemes predicted the turbulent kinetic energy better than the Power-law discretization scheme. It is noteworthy that the results of second order upwind and QUICK were similar. Therefore, second order upwind was used in subsequent simulation in view of the fact that QUICK is more computationally demanding and that the simulations could not reach convergence easily.

4.2 Grid independency

In order to ensure that the solution is independent of grid density, preliminary simulations were carried out, based on the grid sizes presented in Table 3.2. For the 45⁰ pitched blade turbine, the predicted values of mean velocities and turbulence quantities with 282776 cells

and 367628 cells were similar, as shown in Appendix B, and the power numbers were 2.28 and 2.29 respectively. Grid independence for the Rushton turbine was achieved with 135065 cells. As it can be seen in Appendix C, the results revealed that the differences in mean velocities were negligible with the 112522 cells and 135065 cells. This is the same grid size as used by Javed et al. (2006). Test runs were also conducted for the 30° pitched blade turbine and the plotted results in Appendix D showed that the solution with mesh sizes of 527968 cells were similar to that of 363994 cells. Their power numbers of 1.29 and 1.28 respectively gave a further indication of the grid independence. The results of the 60° pitched blade turbine geometry attained grid independence with 507539 cells, which is comparable with the grid size of 451094 cells as shown in Appendix E.

4.3 Mean Velocities and Turbulent Kinetic Energy Profile of 45° Pitched Blade Turbine

The axial velocities in most regions of the tank were in good agreement with the experimental data based on the low error values, except at the level close to the liquid surface ($Z/R = 1.62667$), which showed a large deviation from the LDA data. This could be attributed to the liquid surface being modelled as a free surface. The present prediction was comparable to the predictions of Sahu et al. (1998).

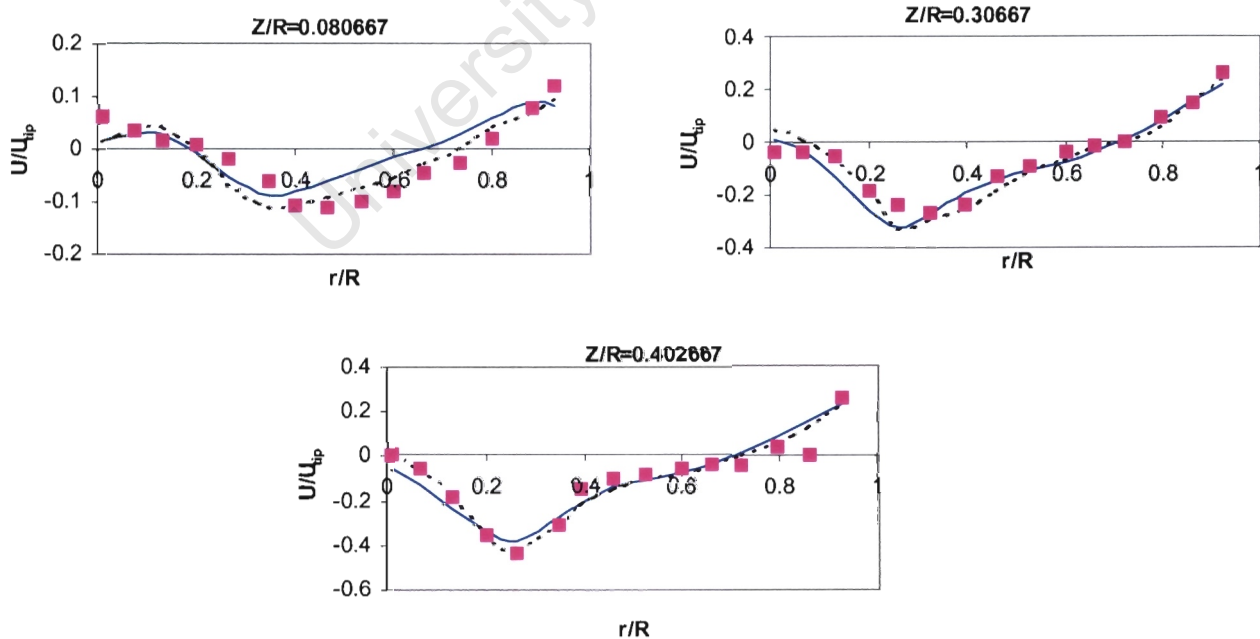


Figure 4:1: Axial velocities below the impeller region: ■ LDA . — Present ---- Sahu 1998

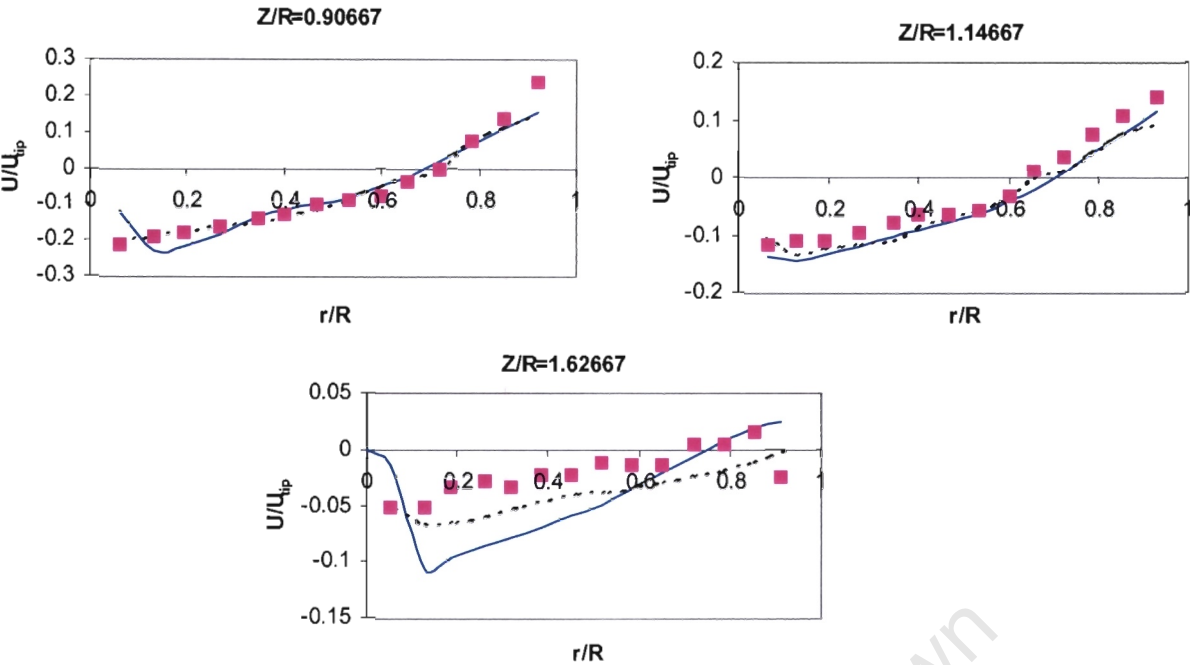


Figure 4:2: Axial velocities above the impeller region: ■ LDA . — Present ---- Sahu 1998

For the CFD radial velocity, there was little or no deviation from the LDA data in most regions of the tank. At $Z/R = 0.90667$, there was a sharp peak in the velocity near the shaft, which was not captured in the experimental data. Ranade (2002), similarly, reported this sharp peak in the downward velocity around the region near the trailing blade, which was not observed in their experimental LDA data. The predictions close to the liquid surface ($Z/R = 1.62667$) were poor as well.

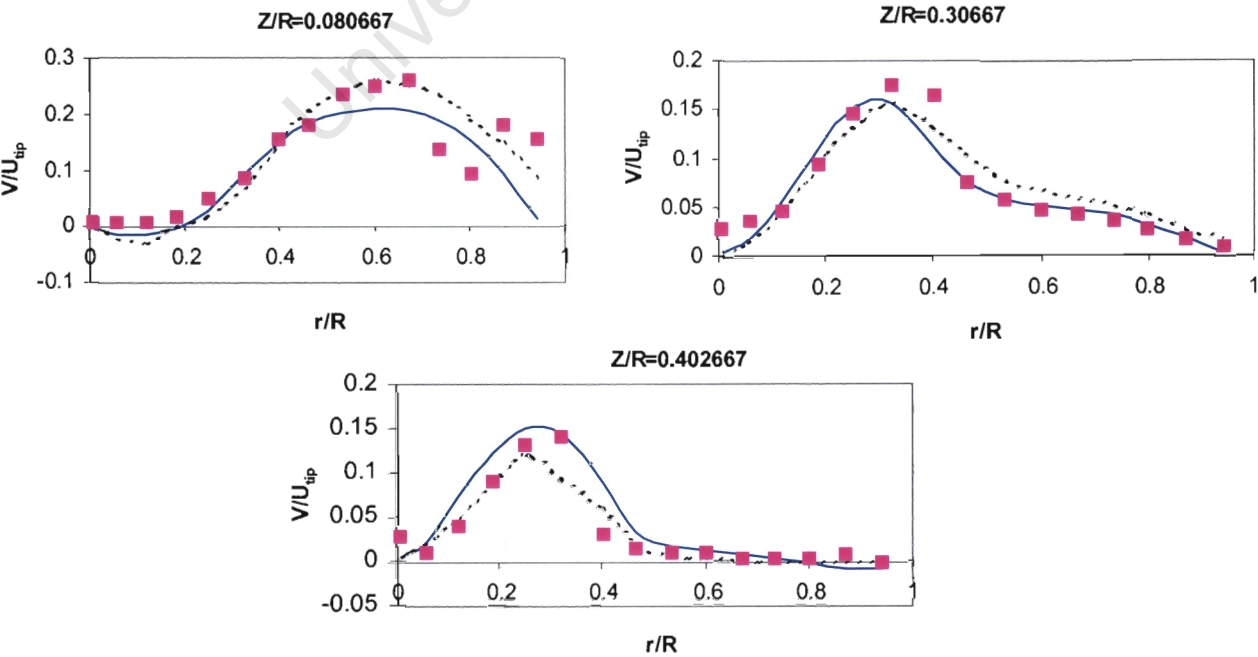


Figure 4:3: Radial velocities below the impeller region: ■ LDA . — Present ---- Sahu 1998

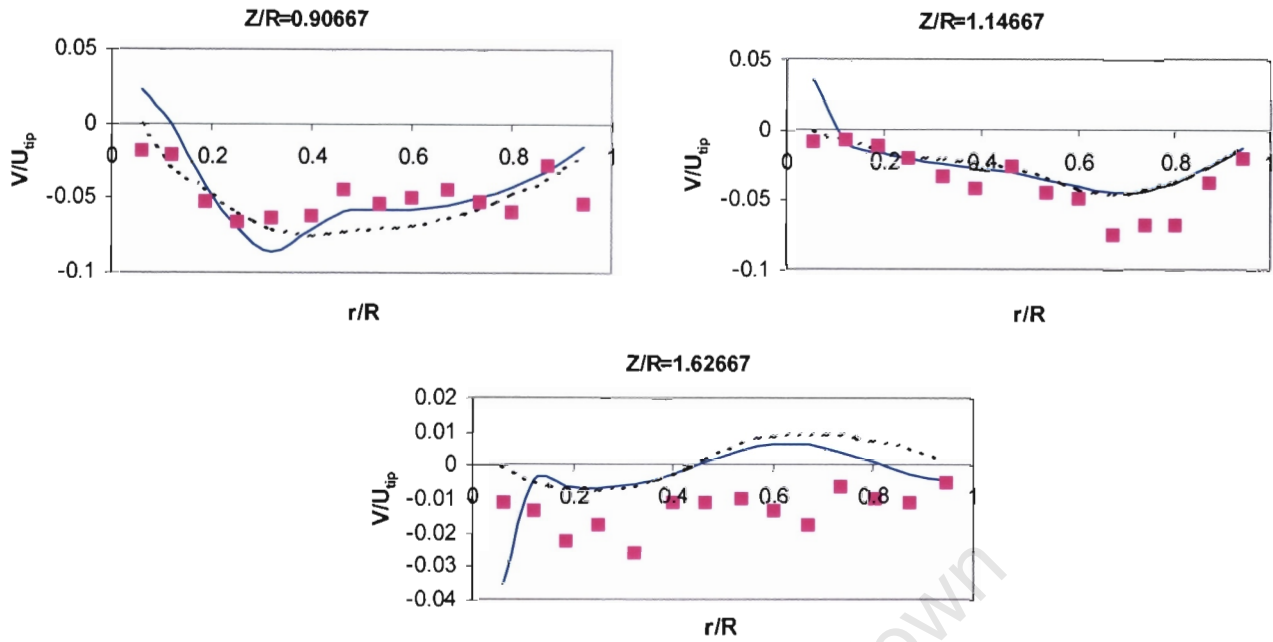


Figure 4:4: Radial velocities above the impeller region: ■ LDA . — Present ---- Sahu 1998

Based on the error values, the CFD tangential velocities were in fairly good agreement with the experimental values, except at some regions in the tank where the predictions were poor. It is interesting to note that the prediction at the level close to the liquid surface ($Z/R = 1.62667$) was in good agreement with the experimental data compared to the axial and radial velocities at this level.

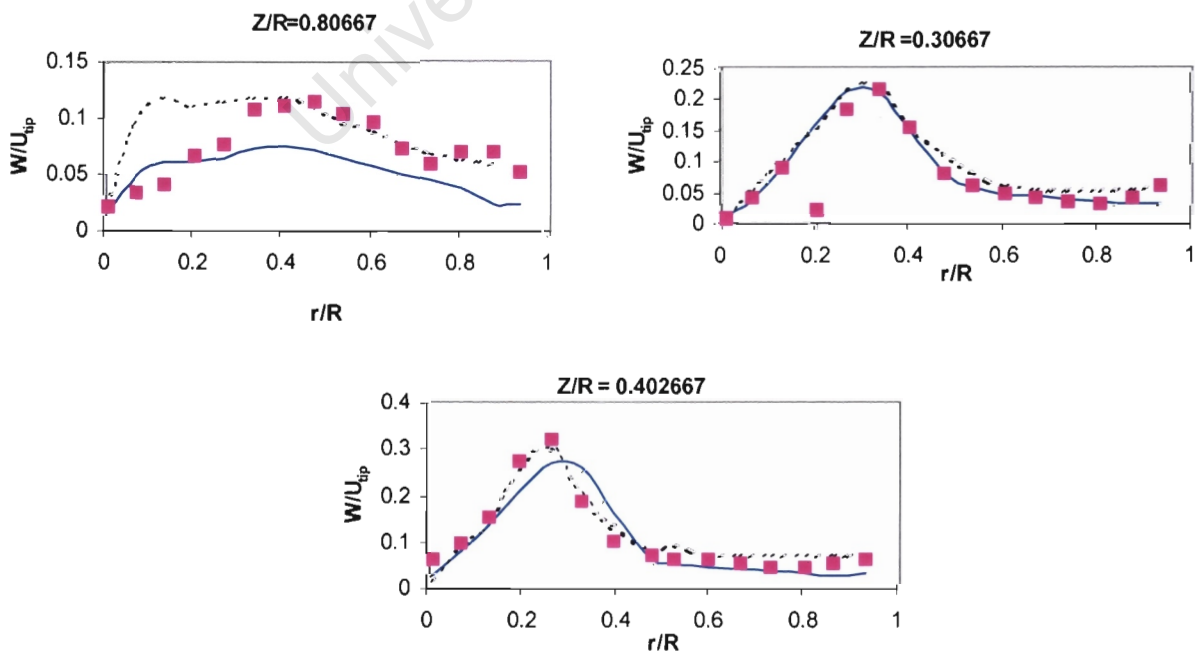


Figure 4:5: Tangential velocities below the tank: ■ LDA . — Present ---- Sahu 1998

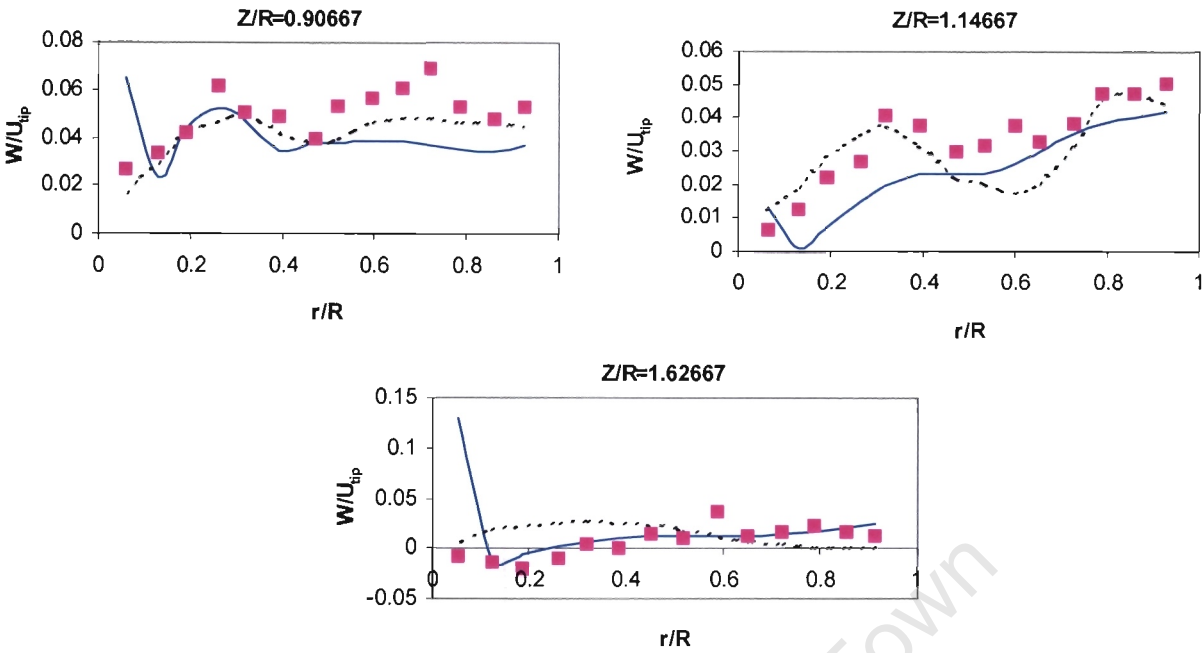


Figure 4:6: Tangential velocities above the impeller region: ■ LDA . — Present
----- Sahu 1998

The turbulent kinetic energy was under-predicted in all the regions of tank. These predictions were compared with those made by Sahu et al. (1998), and it was found that their predictions at the impeller region were better than those of the present model. This can be attributed to the difference in the modelling techniques. Sahu et al. (1998) adopted the black box approach, where the impeller is simulated by providing boundary conditions on an imaginary surface surrounding the impeller. These boundary conditions have to be measured experimentally for the specified geometry. In contrast, the present study employed the Multiple Frame of Reference (MFR) approach discussed earlier (see Section 2.5.1.). Both model predictions did not predict the turbulent kinetic energy quantitatively in the tank. It should be noted that the comparison with Sahu et al. (1998) is to ascertain the performance of the present model prior to the parametric studies.

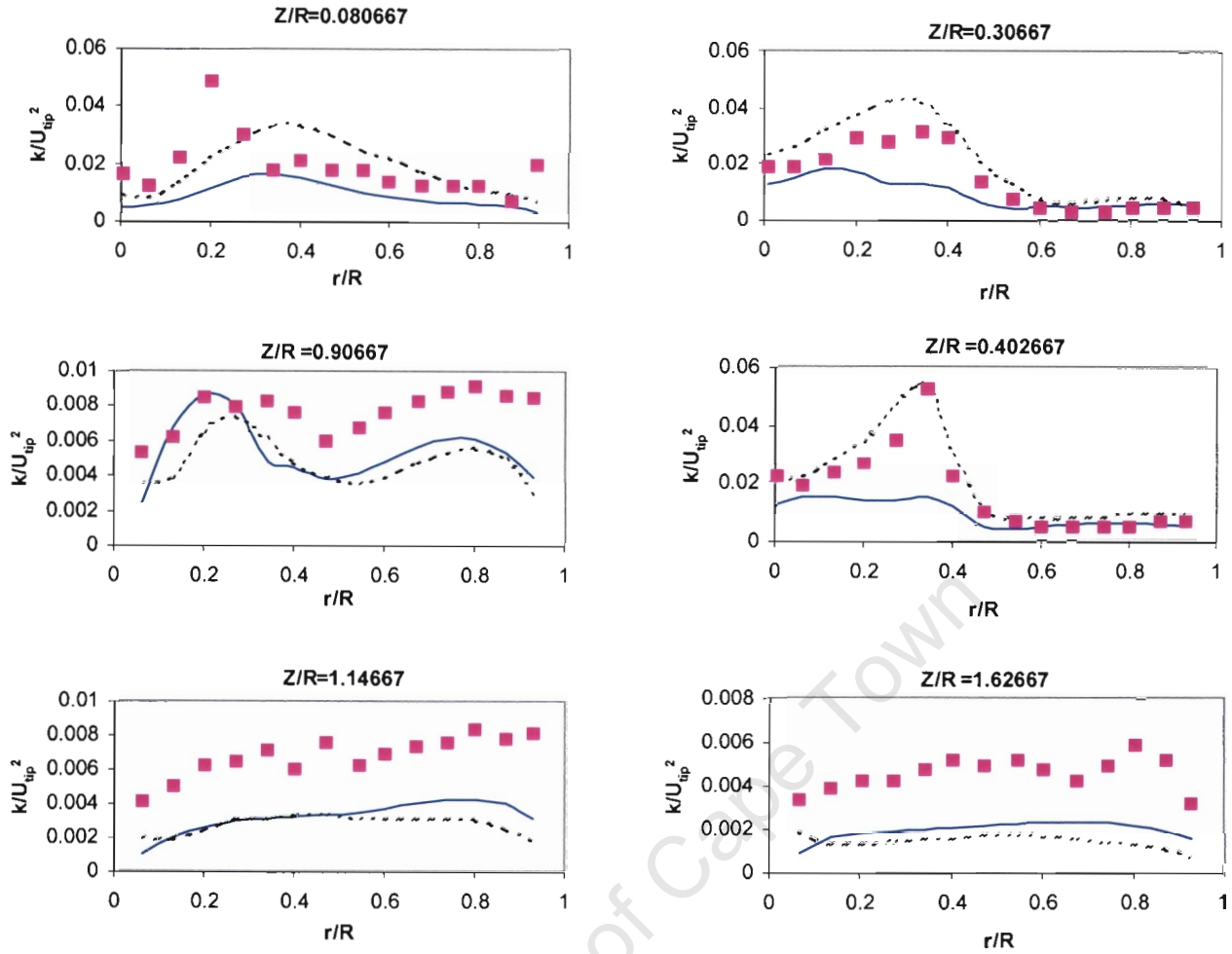


Figure 4:7: Turbulent kinetic energy at different levels of the tank: ■ LDA . — Present
 ---- Sahu 1998

4.4 Parametric analysis

To achieve the aim of the study (viz. to explore the possibility of a suitable set of parameters for the stirred tank reactors), simulations were carried out at different values of C_μ , $C_{\epsilon 1}$ & $C_{\epsilon 2}$, as stated in Tables 3.4, 3.5, 3.6 and 3.7. Consequently, the error values and power number were calculated for each combination of parameters using the approaches earlier discussed in Section 3.7.1. There was consistency in the error values determined. As a result, the error values based on standard error of estimate approach were presented. In the present geometry, the experimental measurements were taken at six levels of the tank in the axial direction and at 15 radial points for each level. This resulted in 90 data points to evaluate the error for each measured quantity. The global error value is the summation of the errors for the mean velocities and the turbulent kinetic energy for each set of combination parameters. It is worth nothing that the ranking of the model parameters in this study is an empirical measure

and is in terms of the error values. The highest ranking is an indication of high error value and poor predictions within the subsets. The ranking of these error values are presented in Appendix F.

The first set of 27 simulations was implemented, and the error values and power numbers are shown in Figure 4.8 and Appendix F. It must be noted that the blue region on Figure 4.8 indicates where the error values are low and this colour code is applicable to other plotted surfaces in this section. It is worth noting that at any C_μ , with a high value of $C_{\varepsilon 2}$ and a low value of $C_{\varepsilon 1}$, the predictions were poor. Based on the error values and power number, good predictions were thus expected at $C_\mu \leq 0.115$. The best prediction with fairly good moment convergence was obtained with the combination $C_\mu = 0.05$, $C_{\varepsilon 1} = 1.25$, $C_{\varepsilon 2} = 2.1$. Moreover, the predicted power number 2.25 at this combination is low compared to the predicted value of 2.28 of the standard $k - \varepsilon$ model and the experimental value of 2.32. The CFD predictions at $C_{\varepsilon 2} = 1.4$ with any other combinations of C_μ and $C_{\varepsilon 1}$ were poor. Similarly, the predictions at $C_{\varepsilon 1} = 1.6$ with any other combination of C_μ and $C_{\varepsilon 2}$ were relatively poor based on the error values.

The trend of results showed that the influence of these parameters cannot be underestimated. In summarizing the solution process for the $k - \varepsilon$ model, transport equations are solved for the turbulent kinetic energy and dissipation rate. The solutions of k and ε are used to calculate the eddy viscosity (μ_t). The results for μ_t and k are used in computing the Reynolds stresses, which is substituted into the RANS equations. After the RANS equations have been solved, the new velocity components are used to update the generation term in the standard $k - \varepsilon$ model and the process is repeated. However, the stability and the determination of other terms in the standard $k - \varepsilon$ model can be affected as result of inappropriate parameters. For instance, the dissipation term in the transport equation for k is simply equal to ε . The turbulent diffusivity of k and ε are related to eddy viscosity with additional empirical parameters, which are known as turbulent Prandtl numbers for k and ε . Rodi (1984) also reported that C_μ is function of the production of turbulent kinetic energy and its dissipation i.e. $C_\mu = f(P/\varepsilon)$. The dependence of other terms in the standard $k - \varepsilon$ model on appropriate parameters cannot be underestimated.

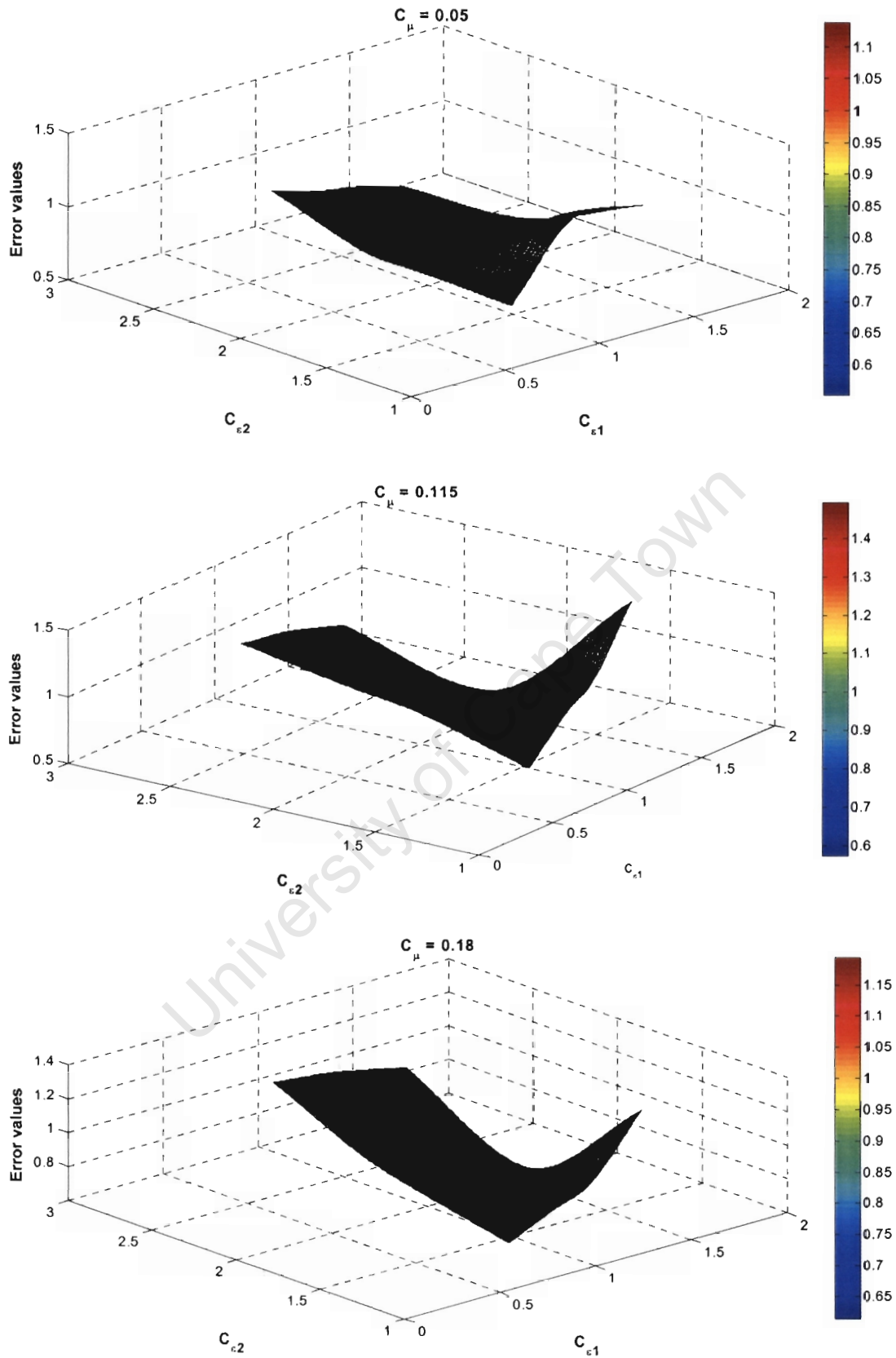


Figure 4:8: The turbulence model parameters and global error values for the first set of simulations (*blue region indicates where the error values are low*)

Based on the findings from the first set of 27 simulations, the combinations of C_μ , $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ were further refined as indicated in Figure 4.9 and Appendix F. The poor moment convergence at $C_\mu = 0.03$ and at all combination of $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ showed that the model parameters are not suitable. However, the lowest error value was obtained with the values of $C_\mu = 0.03$, $C_{\varepsilon 1} = 1.2$, $C_{\varepsilon 2} = 2.2$, the poor moment convergence rendered the model unstable. The results were further analysed at $C_\mu = 0.1$ and at $C_{\varepsilon 1} = 1.2$, $C_{\varepsilon 2} = 1.8$, best prediction was obtained, based on the error values but the moment did not converge. The error value was low for $C_{\varepsilon 1} = 1.4$ and $C_{\varepsilon 2} = 1.8$ and the moment converged. However, the calculated Power number of 2.82 from the converged moment value was higher than the experimental Power number and the predicted value of the standard $k-\varepsilon$ model, which makes the model inappropriate for the system. All other combinations of $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ at $C_\mu = 0.1$ were unstable and unable to predict the flow field accurately. Furthermore, the predictions at $C_\mu = 0.065$ were promising based on the numerical and moment convergence. Good moment convergence and excellent prediction with respect to the error values was obtained for $C_{\varepsilon 1} = 1.2$ and $C_{\varepsilon 2} = 1.8$. In addition, good moment convergence was achieved at $C_{\varepsilon 1} = 1.4$, $C_{\varepsilon 2} = 2.6$, but the error value was high. It was also observed that at any C_μ , in the second set of simulations with a high $C_{\varepsilon 2}$ and a low $C_{\varepsilon 1}$ or vice-versa resulted in poor predictions. The predictions at any C_μ , for $C_{\varepsilon 1} = 1.2$ and $C_{\varepsilon 2} = 1.8$ compared reasonably with the experimental data, but at $C_\mu = 0.03$ or 0.1 , the moment convergence was not achieved. The error values at any C_μ , for $C_{\varepsilon 1} = 1.4$ and $C_{\varepsilon 2} = 1.8$ were high.

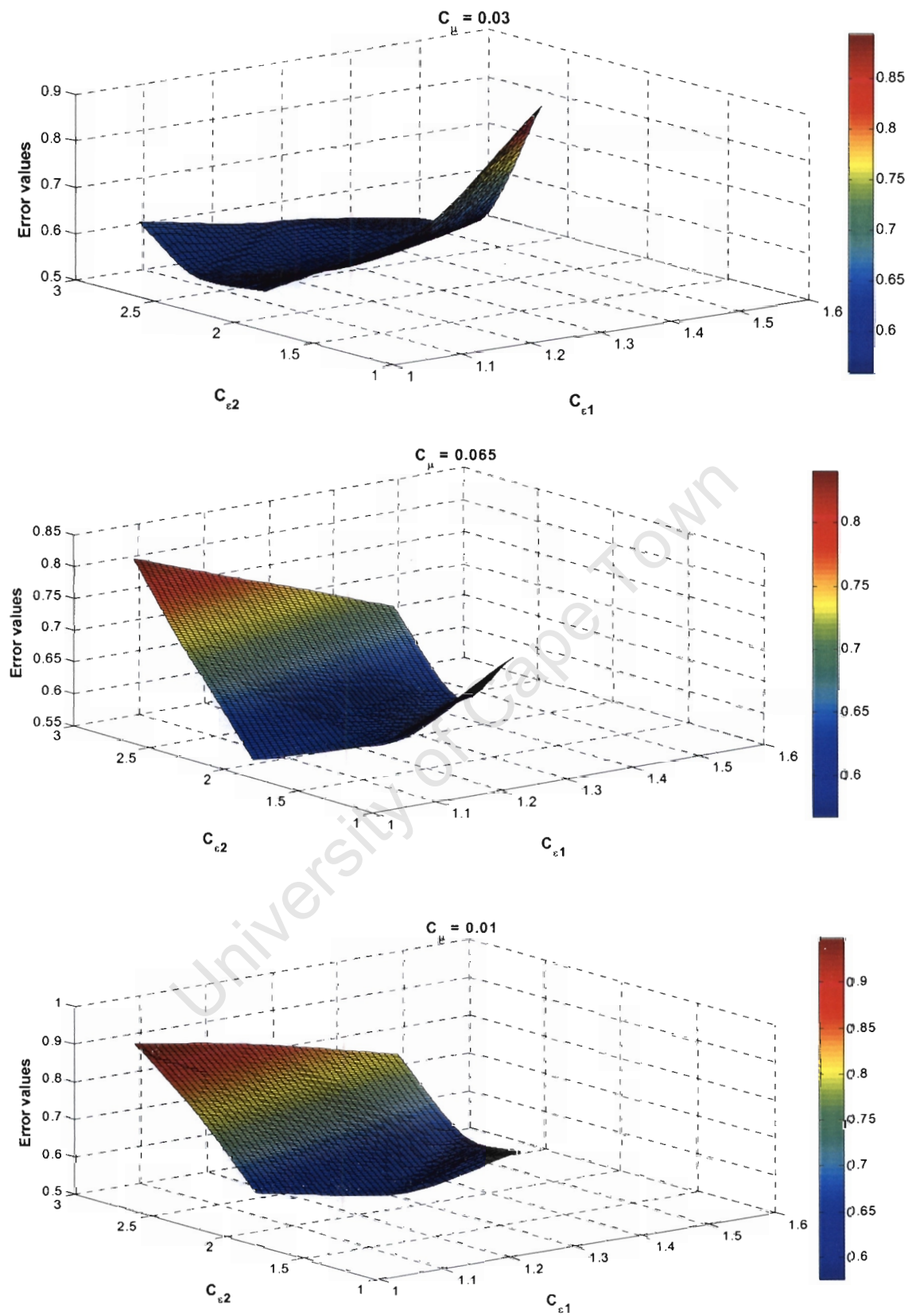


Figure 4:9: The turbulence model parameters and global error values for the second set of simulations (blue region indicates where the error values are low)

As a result of these previous simulations, the model parameters were further refined and the results were plotted in Figure 4.10. The predictions at $C_{\mu} = 0.095$ were poor based on the error values and moment convergence. Nevertheless at $C_{\varepsilon 1} = 1.4$, $C_{\varepsilon 2} = 2$, the predictions were reasonable and the moment convergence was fairly good. It is interesting to note that the predictions were poor at high $C_{\varepsilon 2}$ with all the combinations in this third set of experiments. At low $C_{\varepsilon 1}$, the results were also poor based on the error values. The best prediction was with $C_{\mu} = 0.045$, $C_{\varepsilon 1} = 1.25$ and $C_{\varepsilon 2} = 2$ with good moment convergence, but the calculated Power number 2.40 was higher than the experimental value 2.32. This over-predicted Power number can result in over-estimating the power consumption for the agitated vessel. The combination of $C_{\mu} = 0.045$, $C_{\varepsilon 1} = 1.4$ and $C_{\varepsilon 2} = 2.2$ resulted in excellent predictions, and good moment convergence was achieved with a Power number 0.04% lower than the predicted value of the standard $k-\varepsilon$ model. At $C_{\mu} = 0.07$, the combination of $C_{\varepsilon 1} = 1.4$, $C_{\varepsilon 2} = 2$ gave good predictions with a very good moment convergence resulting in the Power number being slightly lower than the standard $k-\varepsilon$ model. Furthermore, all C_{μ} , with the combination of $C_{\varepsilon 1} = 1.25$, $C_{\varepsilon 2} = 2$, resulted in excellent predictions but the moment converged only when $C_{\mu} = 0.045$.

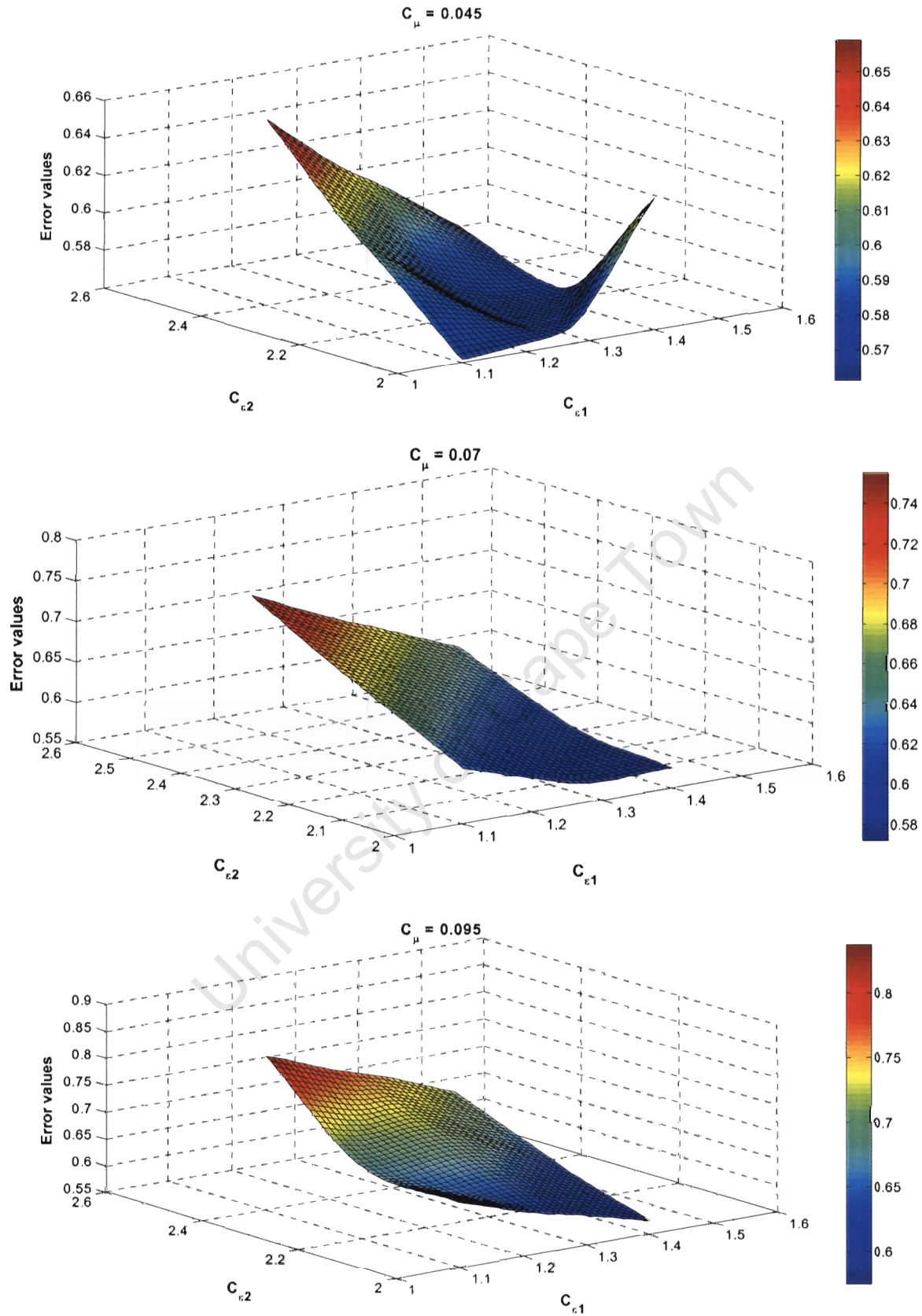


Figure 4:10: The turbulence model parameters and global error values for the third set of simulations (*blue region indicates where the error values are low*)

Considering the results obtained from the third set of simulations, there was an indication that the suitable set of parameters falls within this range. Further simulations were carried out and error values were plotted in Figure 4.11 and Appendix F. The study established that the combination of parameters at low $C_{\epsilon 1}$ and high $C_{\epsilon 2}$ in this set of simulations were not suitable for the stirred tank reactors. Furthermore, at $C_{\mu} = 0.0675$ or 0.09 with $C_{\epsilon 1} = 1.39$, $C_{\epsilon 2} = 2.15$, the predictions were poorer than the standard $k-\epsilon$ model predictions, and the moment convergence was poor. However, at $C_{\mu} = 0.045$ with the same combination of parameters $C_{\epsilon 1}$ and $C_{\epsilon 2}$, the predictions were good based on the error values, and there was a good moment convergence. The predictions at $C_{\epsilon 1} = 1.39$, $C_{\epsilon 2} = 1.95$ and for any C_{μ} were reasonable in terms of the error values but the moment convergence was poor. In addition, at low $C_{\epsilon 2}$ and high $C_{\epsilon 1}$ there was a larger disparity in the experimental values and the predictions compared to the standard $k-\epsilon$ model predictions, which means that the parameters are unsuitable for the system. In analysing the predicted values at $C_{\epsilon 1} = 1.31$, $C_{\epsilon 2} = 1.95$ and $C_{\mu} = 0.0675$ or 0.045 , the results were good but the Power numbers were under-predicted while at $C_{\mu} = 0.09$, the results and moment convergence were poor. The moment convergence was fairly good at $C_{\mu} = 0.09$ or 0.0675 , $C_{\epsilon 1} = 1.22$ and $C_{\epsilon 2} = 1.75$ but at $C_{\mu} = 0.045$ with the same combination of $C_{\epsilon 1}$ and $C_{\epsilon 2}$, the moment convergence was poor. The moment convergence obtained with the combination of parameters $C_{\epsilon 1} = 1.22$, $C_{\epsilon 2} = 1.95$ and $C_{\mu} = 0.045$ was also fairly good.

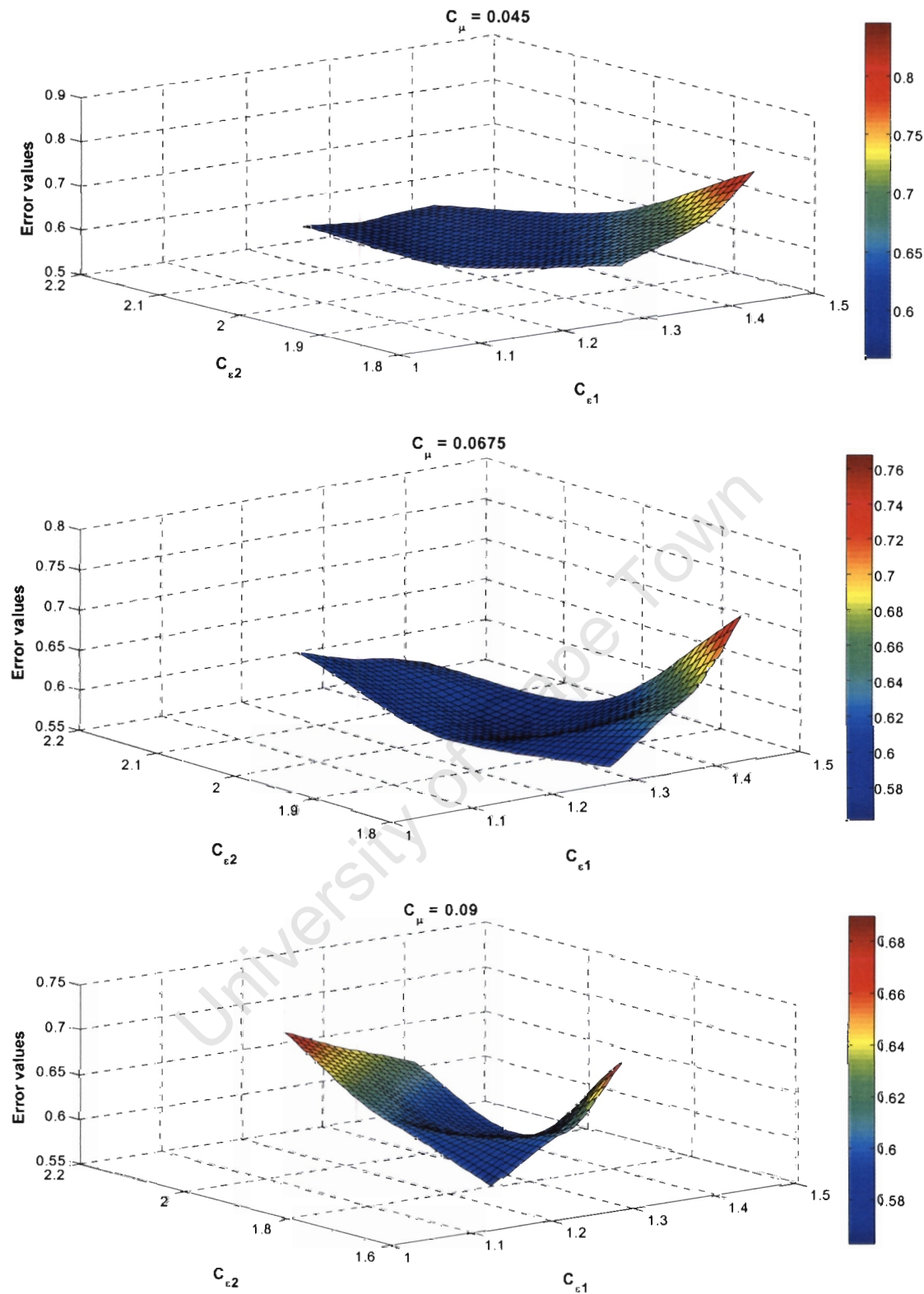


Figure 4:11: The turbulence model parameters and global error values for the fourth set of simulations (*blue region indicates where the error values are low*)

It must be noted that out of the 104 simulations, only 11 combinations presented in Table 4.1 satisfied the stability test approach and low error values. Some combinations of parameters had very low error values but were unstable for stirred tank reactors. For example, the combination $C_\mu = 0.03$, $C_{\varepsilon 1} = 1.2$, $C_{\varepsilon 2} = 2.2$ resulted in lower error values than the standard $k - \varepsilon$ model but the moment convergence was poor. This stability test approach facilitated the elimination of some combinations with the same condition. Further investigation showed that the model parameters with high error values grossly either under or over-predicted the Power number, as plotted in Figure 4.12. The Power number is a key design objective that cannot be under-estimated. Its accurate prediction determines the optimal economics of the agitated vessels by avoiding the over or under-estimation of the power consumed.

Ajayi and Musonge (2006) proposed an optimum range presented in Table 4.2. However, it is worth noting that not all combinations of the parameters within this range will satisfy the two constraints established in the present study. This optimum range contrasts with the modified set of parameters used by Ranade and Joshi (1989). The authors established that Abuejale and Lilley's (1984) set of parameters for recirculating flows are not suitable for stirred tank reactors, as it resulted in poor numerical and moment convergence. In comparison with other parametric studies, the optimum range is within the range in which Sahu et al. (1998) carried out their simulations. There was an indication that all the parameters had a significant effect on the flow field, which is in contradiction to the findings of Nere et al. (2001), suggesting that a variation in $C_{\varepsilon 1}$ and $C_{\varepsilon 2}$ led to relative insensitivity to flow predictions. Nere et al.'s (2001) study reported that a higher value C_μ resulted in an excellent prediction of the flow field when compared to the standard $k - \varepsilon$ model. The results of Ajayi and Musonge (2006) are, however, in contrast with their findings. The numerical convergence was poor at higher C_μ and this makes it unsuitable for stirred tank reactors.

Table 4.1: The optimum turbulence model parameters, error values and Power number

C_μ	$C_{\epsilon 1}$	$C_{\epsilon 2}$	U_{error}	V_{error}	W_{error}	K_{error}	Total Error	Power Number (N_p)	Power (Nm/s)
0.045	1.22	1.95	0.23115	0.14260	0.16460	0.03099	0.56934	2.29	2.85
0.045	1.31	2.15	0.22407	0.14694	0.16020	0.03023	0.56144	2.27	2.83
0.045	1.39	2.15	0.23056	0.14467	0.16671	0.03099	0.57293	2.28	2.84
0.045	1.25	2	0.22800	0.14389	0.16358	0.03083	0.56630	2.40	2.99
0.045	1.4	2.2	0.22737	0.14479	0.16497	0.03052	0.56765	2.28	2.84
0.05	1.25	2.1	0.22614	0.15178	0.15604	0.03129	0.56525	2.25	2.81
0.065	1.2	1.8	0.22737	0.14165	0.16234	0.03623	0.56760	2.29	2.86
0.0675	1.31	1.95	0.22416	0.14407	0.16041	0.03593	0.56456	2.27	2.84
0.07	1.4	2	0.22925	0.14343	0.16457	0.03738	0.57463	2.27	2.84
0.09	1.22	1.75	0.22047	0.14344	0.15852	0.04068	0.56311	2.28	2.85
0.09	1.39	1.95	0.22472	0.14499	0.15981	0.04021	0.56972	2.27	2.83
Standard k – ϵ model			0.24313	0.14304	0.16850	0.04295	0.59762	2.28	2.84

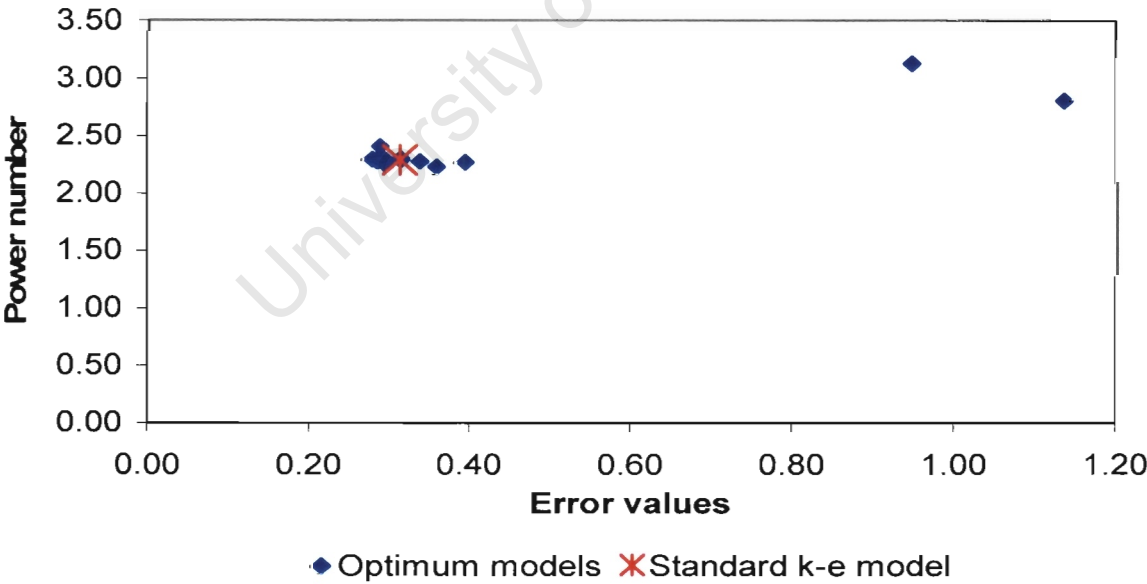


Figure 4:12: Effect of model stability on Power number

Table 4.2: The range of parameters

	C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$
Ajayi and Musonge (2006)	0.045– 0.09	1.2 – 1.4	1.8 – 2.2
Abuejale and Lilley (1984)	0.125	1.44	1.6
Sahu et al. (1998)	0.25 – 0.125	1 – 1.4	1.5 – 2.7
Nere et al. (2001)	0.02 – 0.17	1.24 – 1.64	1.55 – 2.12

A further comparison of the optimum combination of parameters with the standard $k-\varepsilon$ model showed that the parameters have little or no effect on the mean velocities predictions, but a significant improvement within a range of 10% to 35% was achieved in the turbulent kinetic energy predictions. Some of the profile plots are presented in Figures 4.13, 4.14, 4.15, 4.16 and Appendix G. In addition, the predicted Power number N_p within the optimum range of parameters and the standard $k-\varepsilon$ model is relatively the same. The simulated vector plots of the standard $k-\varepsilon$ model and the optimum combination of parameters are presented in Figure 4.17(a) –(d). The plots showed similar flow patterns and the discharge angles of the impeller stream are also analogous.

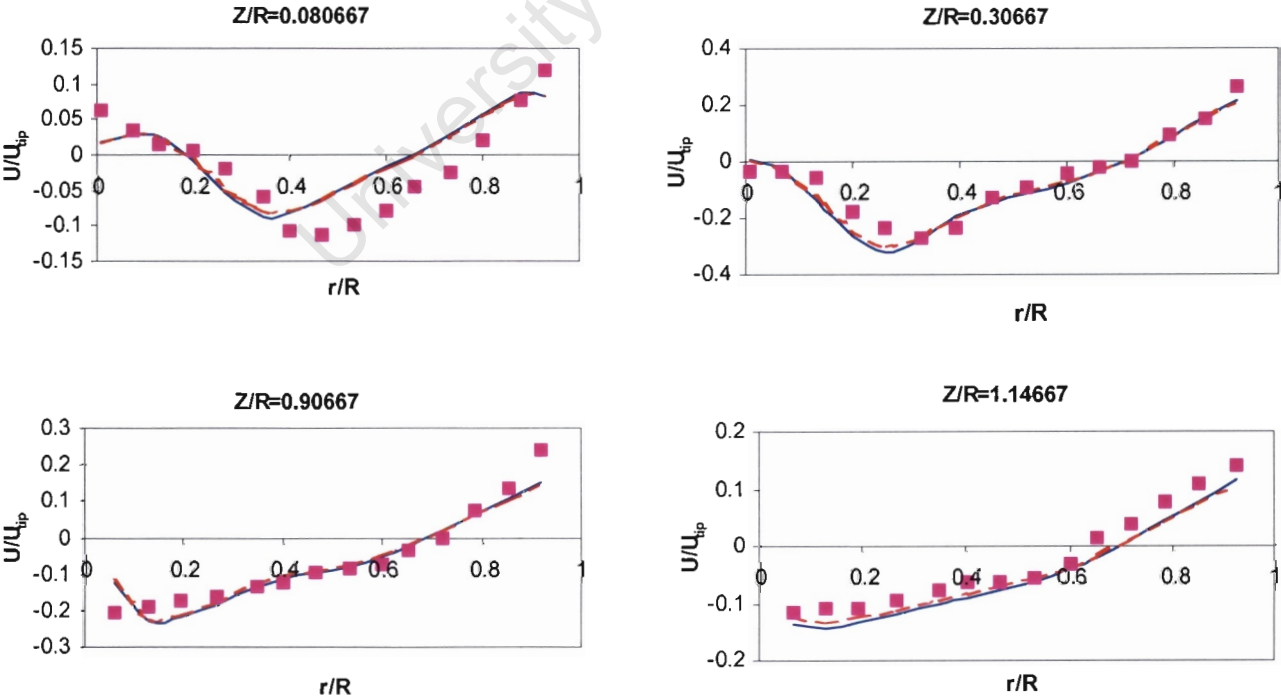


Figure 4.13: Axial velocities of 45° pitched blade turbine with model parameters $C_\mu = 0.065$ $C_{\varepsilon 1} = 1.2$, $C_{\varepsilon 2} = 1.8$: ■ LDA. — Standard $k-\varepsilon$ model. - - - Optimum model parameters

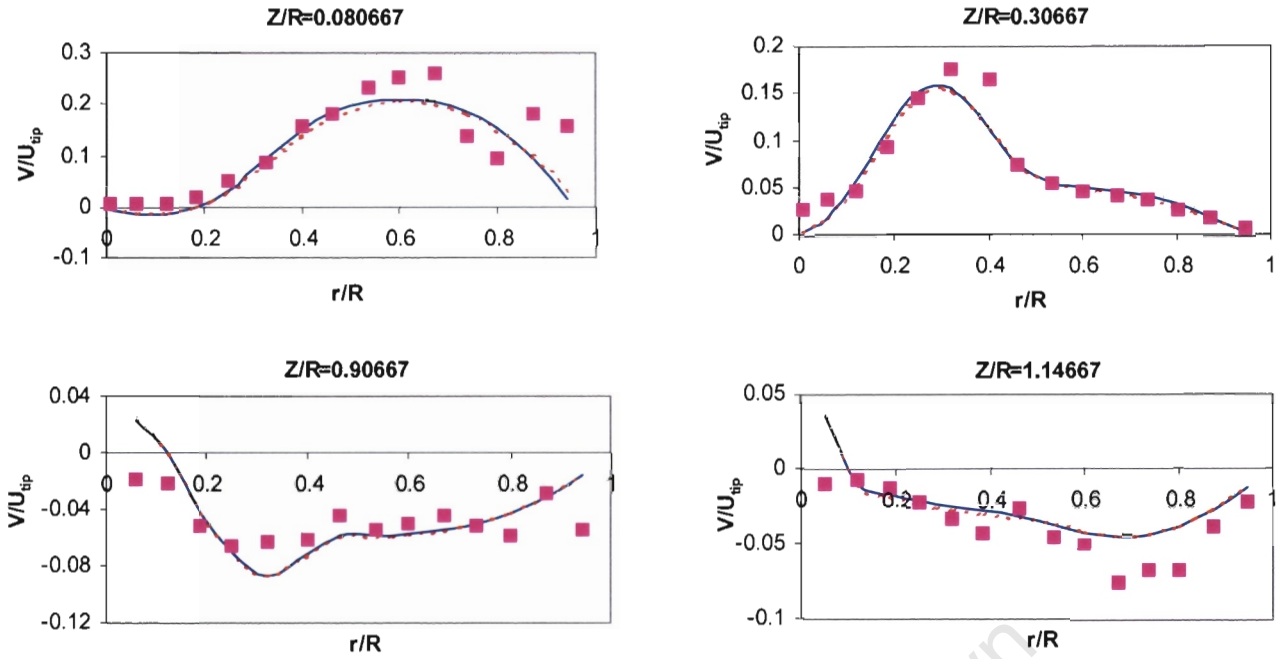


Figure 4:14: Radial velocities of 45° pitched blade turbine with model parameters $C_\mu = 0.065$ $C_{\epsilon 1} = 1.2$, $C_{\epsilon 2} = 1.8$: ■ LDA. — Standard $k-\epsilon$ model. - - - Optimum model parameters

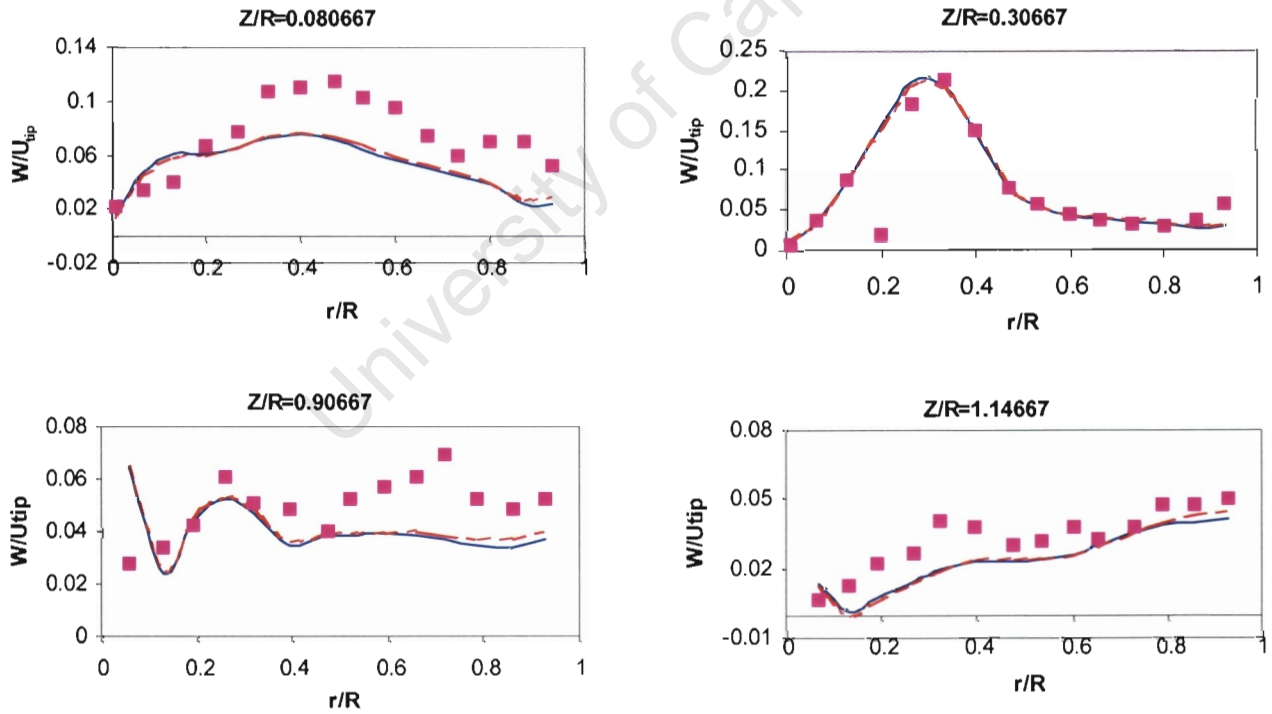


Figure 4:15: Tangential velocities of 45° pitched blade turbine with model parameters $C_\mu = 0.065$, $C_{\epsilon 1} = 1.2$, $C_{\epsilon 2} = 1.8$: ■ LDA. — Standard $k-\epsilon$ model - - - Optimum model parameters

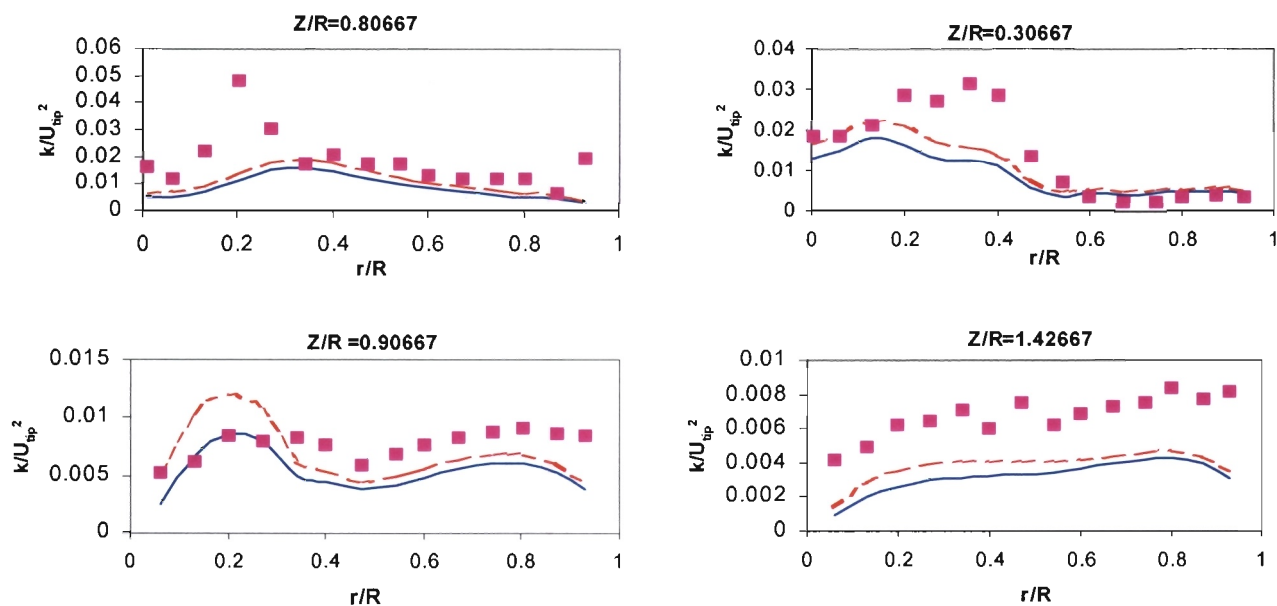


Figure 4:16: Turbulent kinetic energy of 45° pitched blade turbine with model parameters $C_\mu=0.065$, $C_{\epsilon 1}=1.2$, $C_{\epsilon 2}=1.8$: ■ LDA. — Standard $k-\epsilon$ model. - - - Optimum model parameters

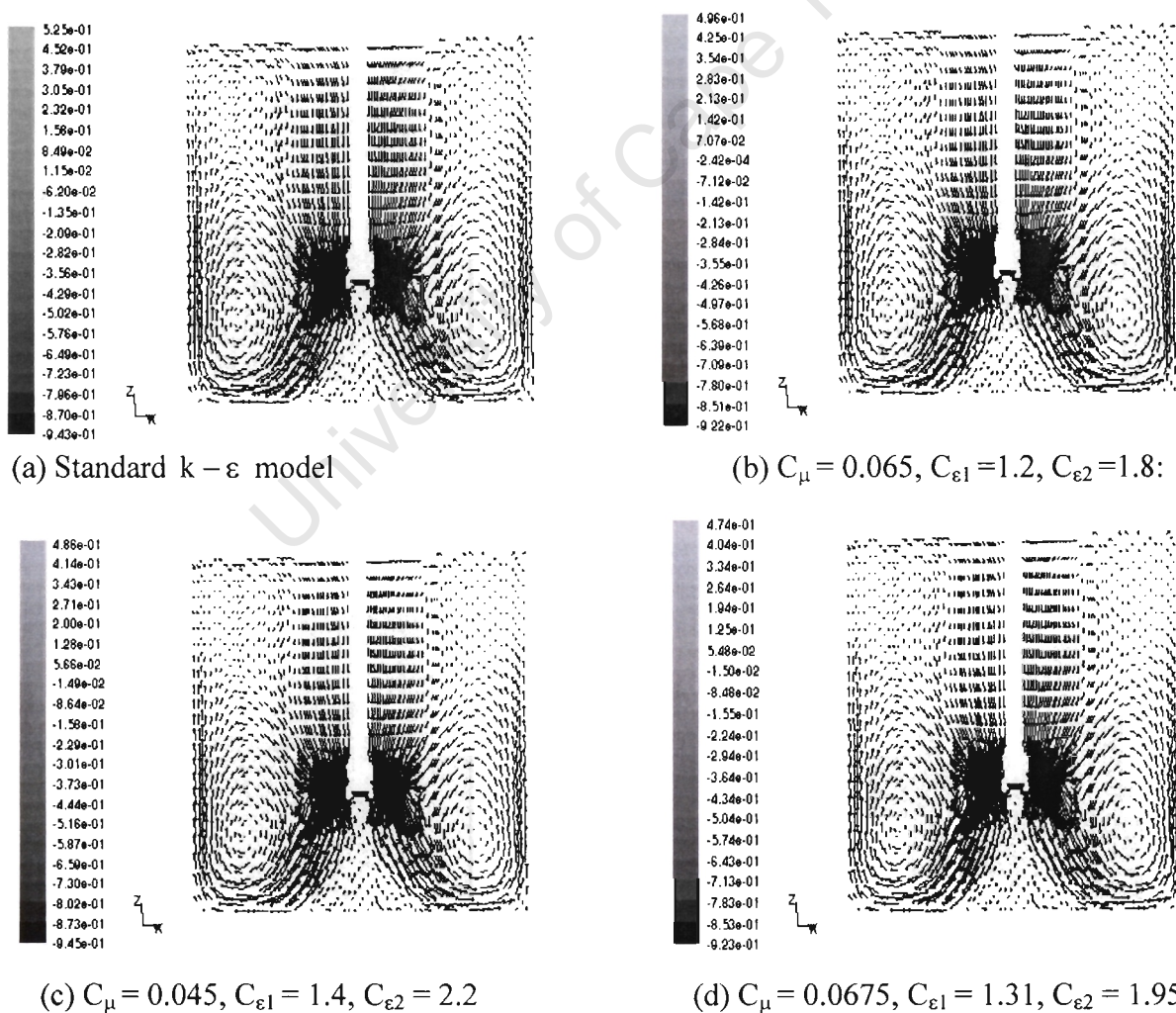


Figure 4:17(a)-(d): Axial velocity vector plots for 45° degree pitched blade

4.5 Examination of the optimum range in case studies

In order to examine the trend of the results within the proposed optimum range of the parameters, simulations were carried out in the three different geometries described in Chapter 3. The error values and Power numbers are presented in Tables 4.3, 4.4, 4.5 and 4.6. The prediction of tangential velocities above the impeller region in the Rushton turbine could not be validated due to lack of experimental data. As a result, the error values for the Rushton turbine stirred tank reactor both below and above the impeller region are presented separately.

Further analysis of the predictions in the axial flow 30° and 60° pitched blade stirred tank reactors showed that the optimum range of parameters has a negligible effect on the mean velocities, although the turbulent kinetic energy was improved quantitatively within the range of 15% - 20% compared to the standard $k - \epsilon$ model as presented in Appendices I and J. It is worth noting that the Power number increased with an increase in the blade angle and vice versa. This phenomenon agrees with the experimental findings of Ranade et al. (1989) and Yeng-Yung et al. (2006). The mean velocities and turbulent kinetic also behaved similarly to the Power number.

For the Rushton turbine, which is a radial flow impeller, the optimum range of parameters has a significant effect on the radial and tangential velocities as plotted in Appendix H, while the predictions of the axial velocities were comparable with the standard $k - \epsilon$ model. The flow in its discharge stream is characterized by the existence of strong radial and tangential components of the mean velocity and intense turbulence, as shown in Figures 4.18, 4.19 and 4.20. The predictions of its turbulent kinetic energy were also improved within a range of 10% to 33%.

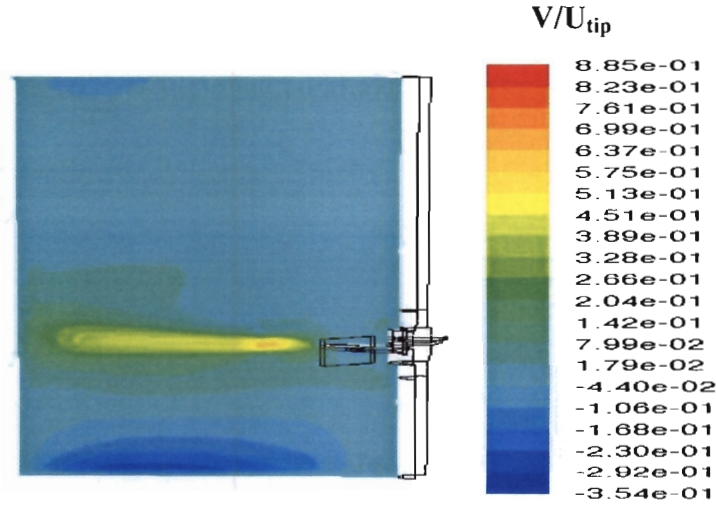


Figure 4:18: Contours of Radial velocity in the Rushton turbine agitated vessel

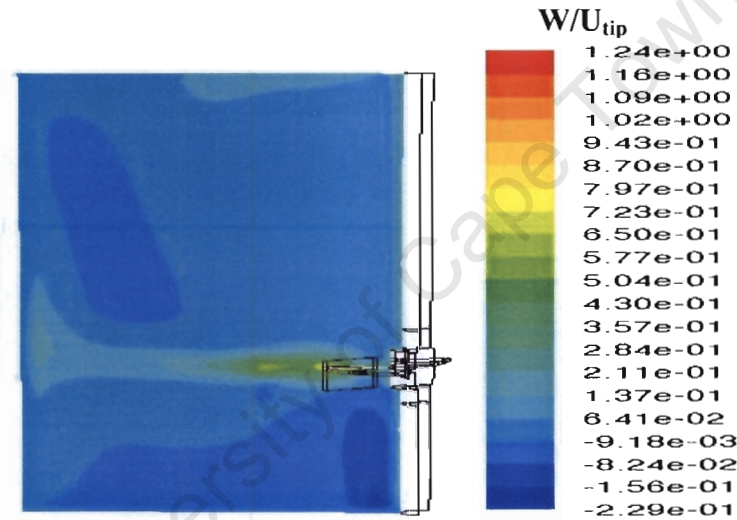


Figure 4:19: Contours of Tangential velocity in the Rushton turbine agitated vessel

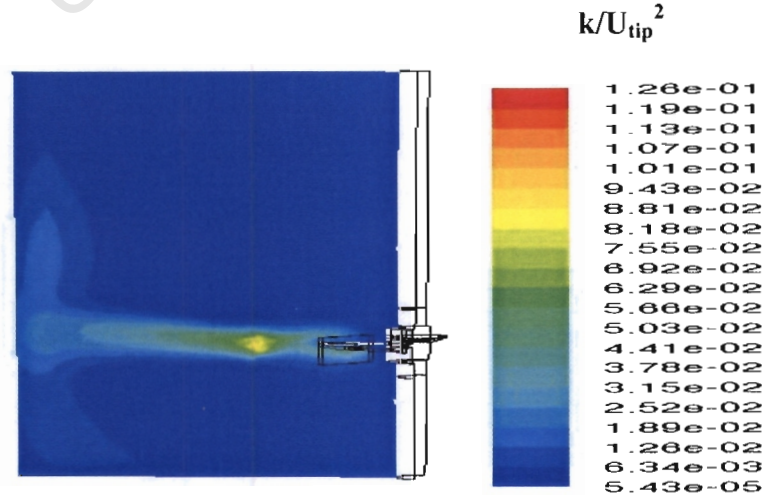


Figure 4:20: Contours of Turbulent kinetic energy in the Rushton Turbine agitated vessel

Table 4.3 The optimum combination of parameters, error values below the impeller region and Power number for the Rushton turbine stirred tank reactor

C_{μ}	$C_{\epsilon 1}$	$C_{\epsilon 2}$	U_{error}	V_{error}	W_{error}	K_{error}	Total error	Power Number (N_p)
0.045	1.22	1.95	0.09282	0.06785	0.09569	0.02094	0.27729	4.00
0.045	1.25	2	0.09455	0.06965	0.08572	0.02054	0.27046	3.99
0.045	1.31	2.15	0.10803	0.08281	0.05501	0.01918	0.26503	3.90
0.045	1.39	2.15	0.09447	0.06938	0.08480	0.02021	0.26886	4.00
0.045	1.4	2.2	0.09914	0.07318	0.06508	0.01966	0.25705	3.97
0.05	1.25	2.1	0.11057	0.10889	0.05200	0.01932	0.29079	3.85
0.065	1.2	1.8	0.09061	0.06627	0.10271	0.02524	0.28482	4.00
0.0675	1.31	1.95	0.09693	0.07217	0.07279	0.02410	0.26599	3.97
0.07	1.4	2	0.09258	0.06781	0.09365	0.02502	0.27906	4.01
0.09	1.22	1.75	0.09224	0.06849	0.09068	0.02762	0.27902	3.99
0.09	1.31	1.95	0.09671	0.07247	0.07148	0.02640	0.26706	3.97
Standard k – ϵ model			0.09082	0.06230	0.12631	0.02891	0.30834	4.06

Table 4.4: The optimum combination of parameters, error values above the impeller region and Power number for the Rushton turbine stirred tank reactor

C_{μ}	$C_{\epsilon 1}$	$C_{\epsilon 2}$	U_{error}	V_{error}	W_{error}	K_{error}	Total error	Power Number (N_p)
0.045	1.22	1.95	0.18518	0.04101	0.00000	0.02467	0.25086	4.00
0.045	1.25	2	0.18804	0.04614	0.00000	0.02412	0.25830	3.99
0.045	1.31	2.15	0.18679	0.06293	0.00000	0.02234	0.27205	3.90
0.045	1.39	2.15	0.18717	0.03869	0.00000	0.02464	0.25050	4.00
0.045	1.4	2.2	0.19189	0.05212	0.00000	0.02339	0.26740	3.97
0.05	1.25	2.1	0.17614	0.06128	0.00000	0.02271	0.26013	3.85
0.065	1.2	1.8	0.18498	0.04276	0.00000	0.02710	0.25485	4.00
0.0675	1.31	1.95	0.18954	0.05504	0.00000	0.02614	0.27072	3.97
0.07	1.4	2	0.18607	0.03807	0.00000	0.02795	0.25209	4.01
0.09	1.22	1.75	0.18701	0.05205	0.00000	0.02651	0.26558	3.99
0.09	1.39	1.95	0.20640	0.07247	0.00000	0.02814	0.30701	3.97
Standard k – ϵ model			0.18345	0.03853	0.00000	0.03151	0.25349	4.06

Table 4.5: The optimum combination of parameters, error values and Power number for 30⁰ pitched blade turbine stirred tank reactor

C_{μ}	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	U_{error}	V_{error}	W_{error}	K_{error}	Total error	Power Number (N_p)
0.045	1.22	1.95	0.24681	0.10754	0.24487	0.02491	0.62413	1.32
0.045	1.25	2	0.24597	0.10729	0.24451	0.02466	0.62243	1.31
0.045	1.31	2.15	0.24177	0.11124	0.24116	0.02324	0.61740	1.29
0.045	1.39	2.15	0.24536	0.10929	0.24056	0.02373	0.61893	1.28
0.045	1.4	2.2	0.24386	0.10847	0.24077	0.02341	0.61652	1.28
0.05	1.25	2.1	0.24362	0.10837	0.24590	0.02404	0.62193	1.31
0.065	1.2	1.8	0.24622	0.11201	0.24241	0.02635	0.62699	1.31
0.0675	1.31	1.95	0.24232	0.10747	0.24126	0.02576	0.61680	1.28
0.07	1.4	2	0.24495	0.10924	0.24043	0.02616	0.62078	1.28
0.09	1.22	1.75	0.24199	0.10703	0.24152	0.02765	0.61820	1.29
0.09	1.39	1.95	0.24278	0.10793	0.24077	0.02715	0.61864	1.28
Standard k – ε model			0.25785	0.04284	0.29226	0.00330	0.59625	1.28

Table 4.6: The optimum combination of parameters, error values and Power number for the 60⁰ pitched blade turbine stirred tank reactor

C_{μ}	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	U_{error}	V_{error}	W_{error}	K_{error}	Total error	Power Number (N_p)
0.045	1.22	1.95	0.48256	0.31781	0.39469	0.05907	1.25413	4.65
0.045	1.25	2	0.48512	0.31955	0.39403	0.05877	1.25748	4.64
0.045	1.31	2.15	0.48874	0.32438	0.38893	0.05795	1.26000	4.59
0.045	1.39	2.15	0.49282	0.32524	0.39918	0.05840	1.27564	4.63
0.045	1.4	2.2	0.49312	0.32648	0.39564	0.05803	1.27327	4.61
0.05	1.25	2.1	0.48545	0.32335	0.38313	0.05799	1.24993	4.57
0.065	1.2	1.8	0.47781	0.31172	0.39213	0.06204	1.24370	4.65
0.0675	1.31	1.95	0.48368	0.31730	0.39008	0.06101	1.25209	4.61
0.07	1.4	2	0.48856	0.31859	0.39713	0.06177	1.26604	4.62
0.09	1.22	1.75	0.47522	0.31045	0.38787	0.06454	1.23808	4.63
0.09	1.39	1.95	0.48495	0.31701	0.39084	0.06336	1.25616	4.61
Standard k – ε model			0.48787	0.31703	0.40664	0.06550	1.27703	4.63

It is interesting to note that the optimum combination of parameters presented in Table 4.1 showed a similar trend in their error values in all the geometries investigated. In view of this, a single combination of parameters was proposed for stirred tank reactors. This was achieved by summing the error values in both the model predictions and the power numbers, which is plotted in Figure 4.21. The model parameters with the least error value were considered suitable for stirred tank reactors. Consequently, the model parameters $C_\mu = 0.065$, $C_{\epsilon 1} = 1.2$, $C_{\epsilon 2} = 1.8$ was found with the lowest error value among the optimum turbulence model parameters. This set of parameters was proposed for predicting the turbulent flow field in stirred tank reactors.

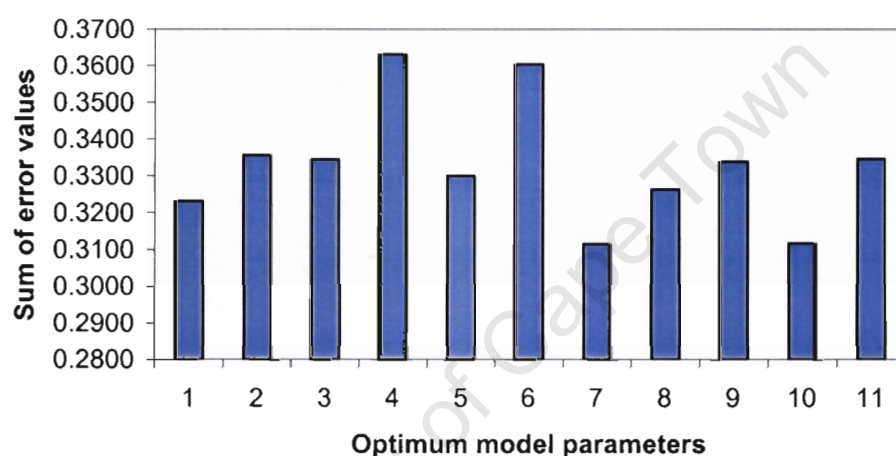


Figure 4:21: Showing the combination of parameters with the Error values

However, a critical examination of the predictions within the optimum range of parameters in all the geometries showed that the turbulent kinetic energy was underestimated throughout the tank. There was also no drastic change in mean velocities in problematic regions of the tank such as the liquid surface. Studies have established that the experimental errors for the mean velocities and turbulent intensity were approximated at $\pm 1\%$ and $\pm 2\%$ respectively (Ranade et al., 1989; Ranade and Joshi, 1990) but the calculated errors were larger than this uncertainty in the experimental data. Consequently, the computed error is not comparable with the experimental error. Several investigations have also reported that the error in LDA measurement techniques is negligible (Montante et al., 2001; Ng et al., 1998). Therefore, the experimental errors do not account for the large discrepancy. Further investigation in the trend of the error values in the mean velocities showed that the predictions close to the wall were poor. The overall error values of mean velocities in the axial direction of the tank are presented in Figure 4.21(a)-(c). These overall error values were calculated by summing all

the calculated deviations in the axial direction of the tank i.e. the direction of the axis with the impeller shaft as point 1 on Figure 4.21.

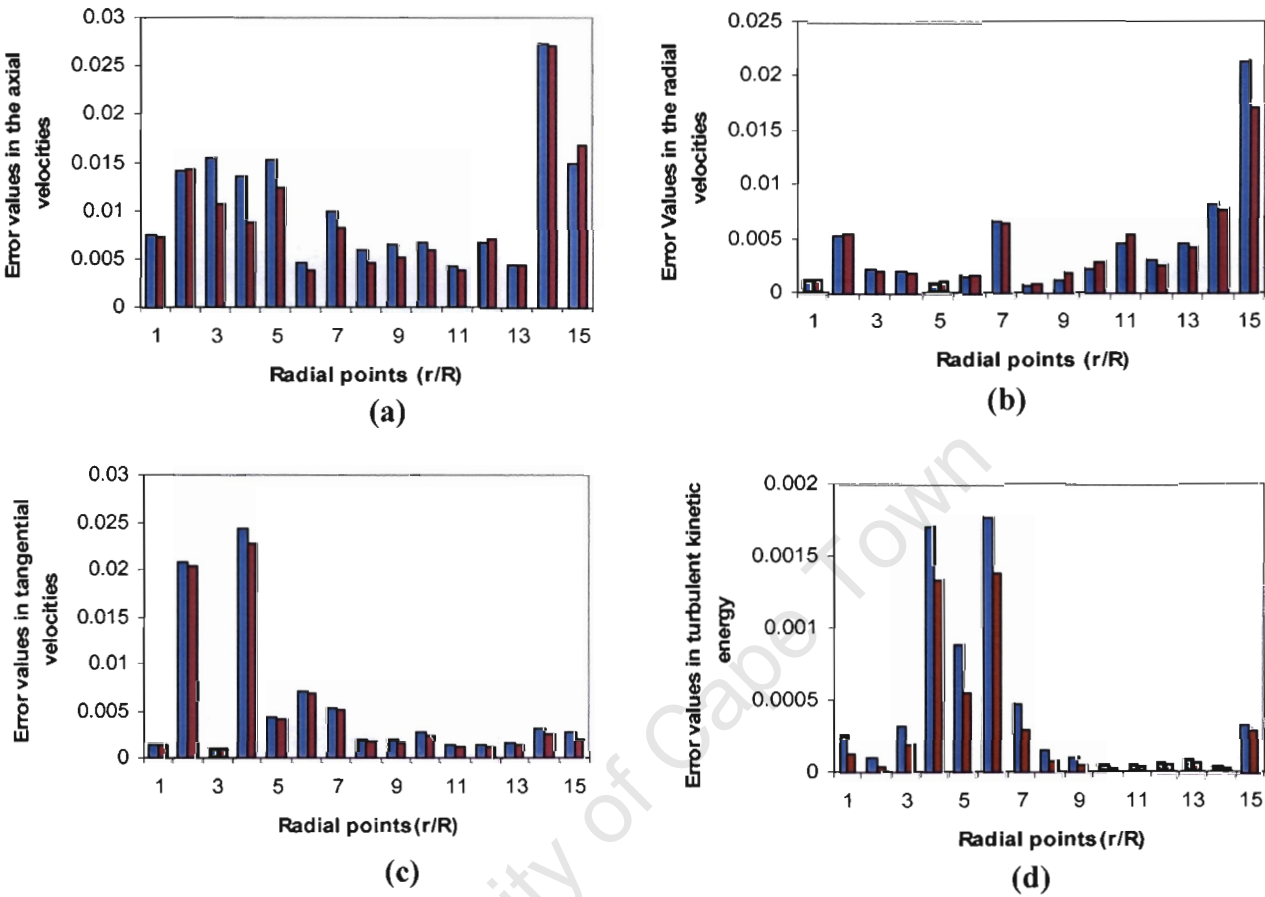


Figure 4:22(a)-(d): The error values in the axial direction of the 45° pitched blade stirred tank reactor: ■ Standard $k-\epsilon$ model. ■ Optimum model parameters ($C_\mu = 0.065$ $C_{\epsilon 1} = 1.2$, $C_{\epsilon 2} = 1.8$)

The high error values can be attributed to the errors involved in the implementation of the wall treatment algorithms and anisotropic flows caused by the baffles. The wall function is valid only when the first grid point adjacent to the wall is within the logarithmic region of the turbulent boundary layer. The dimensionless distance from the wall y^+ should be within a defined recommended range of 30 - 300. However, it is difficult to establish that y^+ is maintained within this range at all the wall boundaries throughout the computation process. The free surface assumption of zero shear stress may also be a contributing factor to the high error values in CFD predictions close to the liquid surface. This assumption does not agree with the reality, where the impeller and the baffles cause the liquid surface to move in the three different directions.

High error values of the turbulent kinetic energy were noticed around the impeller region as illustrated in Figure 4.21(d). Experimental measurements have revealed that there is turbulence anisotropy around the impeller region (Harvey and Greaves, 1982; Lee and Yianneskis, 1998; Hockey and Nouri, 2000). This phenomenon is contrary to the isotropic assumption of the standard $k-\epsilon$ model and it may be responsible for the discrepancy due to the fact that the model performs poorly in highly anisotropic flows. The standard $k-\epsilon$ model is also known to perform excellently in fully turbulent flows like a pipe flow with high Reynolds number. However, Figures 4.20 and 4.22 have shown that turbulent kinetic energy is only high around the impeller region due to the large velocity gradient, but away from this region, the bulk flow has low turbulence intensity.

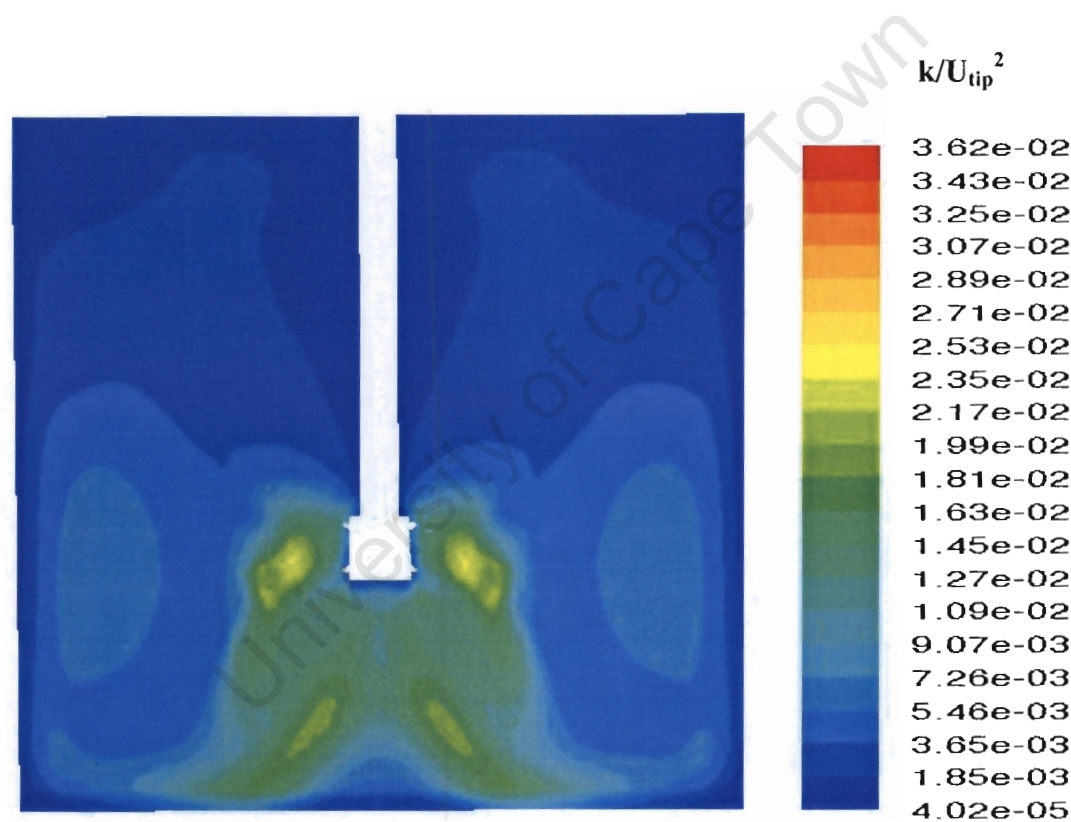


Figure 4:23: Contours of turbulent kinetic energy in the 45° pitched blade turbine agitated vessel

This assumption of the same level of turbulence throughout the tank may also account for the mismatch. There is a possibility that the flow around the impeller region is turbulent while away from the impeller, a laminar regime may be experienced. Ng et al. (1998) have also expressed uncertainty about the LDA measurements around the impeller region. All these

factors may be responsible for the discrepancy between the experiment measurements and the predictions, rather than the unsuitability of the parameters in the standard $k - \varepsilon$ model.

CHAPTER 5

5 CONCLUSIONS AND RECOMMENDATIONS

The accurate prediction of the hydrodynamics in the stirred tank reactors is vital to its proper design and understanding of the mixing mechanism.

5.1 Conclusions

The following conclusions are drawn from the investigation of the performance of the standard $k - \epsilon$ model in predicting the flow field in the agitated vessel:

- Preliminary simulations were carried out to determine the effect of discretization on the predictions. It was established that the choice of discretization schemes has very little effect on predicting the mean velocities but a significant effect on predicting the turbulent kinetic energy. The second order upwind scheme and QUICK (a third order differencing scheme) gave similar results. The second order upwind discretization scheme was employed in subsequent simulations.
- As reported in the literature, the present study established that the standard $k - \epsilon$ model reasonably predicted the mean velocities but the turbulent kinetic energy was quantitatively under-predicted throughout the tank.
- Grid refinements did not resolve the mismatch between the predictions and the experimental data.
- The present work provides a tool for quantifying the errors obtained between predictions and experiments.
- Achieving the aim of the present study, which was exploring the possibility of a suitable set of parameters in the standard $k - \epsilon$ model, resulted in an optimum range of parameters.
- The optimum range was achieved by ensuring the stability of the model and the least deviation from the experimental data. These approaches have not been combined together in previous parametric studies.
- However, it should be noted that not all combinations of the parameters within the range would satisfy the two established constraints employed in this study.
- The optimum range gave better predictions than the standard $k - \epsilon$ model based on the estimated overall error values between the predictions and the experimental data.

- This optimum range contrasts with the Abuejela and Lilley's (1984) set of parameters for recirculating flows used by Ranade and Joshi (1989) and found it unsuitable for stirred tank reactors, as it resulted in poor numerical and moment convergence.
- There was an indication that all the parameters had a significant effect on the flow field, which in contrast with the findings of Nere et al. (2001), suggesting that a variation in $C_{\epsilon 1}$ and $C_{\epsilon 2}$ led to relative insensitivity to flow predictions.
- An in-depth analysis showed that the optimum range of parameters has a negligible effect on the mean velocities in 30° , 45° and 60° pitched turbine agitated vessels, but an improvement of 10% to 35% was achieved in their predictions of the turbulent kinetic energy.
- In the Rushton turbine, the optimum range of parameters has a noticeable effect on the radial and tangential velocities but the predictions of the axial velocities were comparable with those of the standard $k-\epsilon$ model. There was furthermore an improvement of 10% to 35% in the prediction of the turbulent kinetic energy.
- It is worth noting that the optimum combination of parameters presented in Table 4.1 showed a similar trend in their error values in all the geometries investigated
- Therefore, the model parameters $C_\mu=0.065$, $C_{\epsilon 1}=1.2$, $C_{\epsilon 2}=1.8$ has been proposed for predicting the turbulent flow field in stirred tank reactors as a result of lowest error value in both the predictions and the power number.
- Although the proposed optimum set provided an accurate representation of the mean flow field, the turbulent kinetic energy was under-predicted in all the investigated geometries.
- The eddy viscosity assumption of isotropy may be responsible for the discrepancy considering the inability of the model to predict accurately the turbulence kinetic energy around the impeller region, where it is expected to perform well.
- The optimum range of parameters did not resolve the poor predictions close to the liquid surface in any of the geometries.
- The predictions of Power number, N_p , within the optimum range and the standard $k-\epsilon$ model parameters are comparable.

5.2 Recommendations

- A critical analysis of the results suggests that the standard $k-\varepsilon$ model should be completely modified for stirred tank reactors not the variation of the parameters in the model as was done in both previous and present studies.
- A suitable set of parameters may be achieved for stirred tank reactors, taking into account that the production of the turbulent kinetic energy is not equal to the energy dissipation in the case of stirred tank reactors. The parameters in the standard $k-\varepsilon$ model were derived based on the assumption that the production and dissipation of the turbulence energy were almost equal. In stirred tank reactors, however, this assumption may not be valid, because the turbulent energy around the impeller is high and away from the impeller region, the turbulence decreases (see Figures 4.20 and 4.22).
- The modification process may require modelling the parameters as a function of the turbulence field.
- The possibility of developing an in-house CFD code should be explored and the results can be validated further with commercial CFD packages. This will allow for greater flexibility in modifying the model, specifically in the case of stirred tank reactors.
- The LDA measurement techniques to determine the turbulent kinetic energy dissipation rate should be improved to avoid uncertainty in the experimental data.

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APPENDICES

APPENDIX A

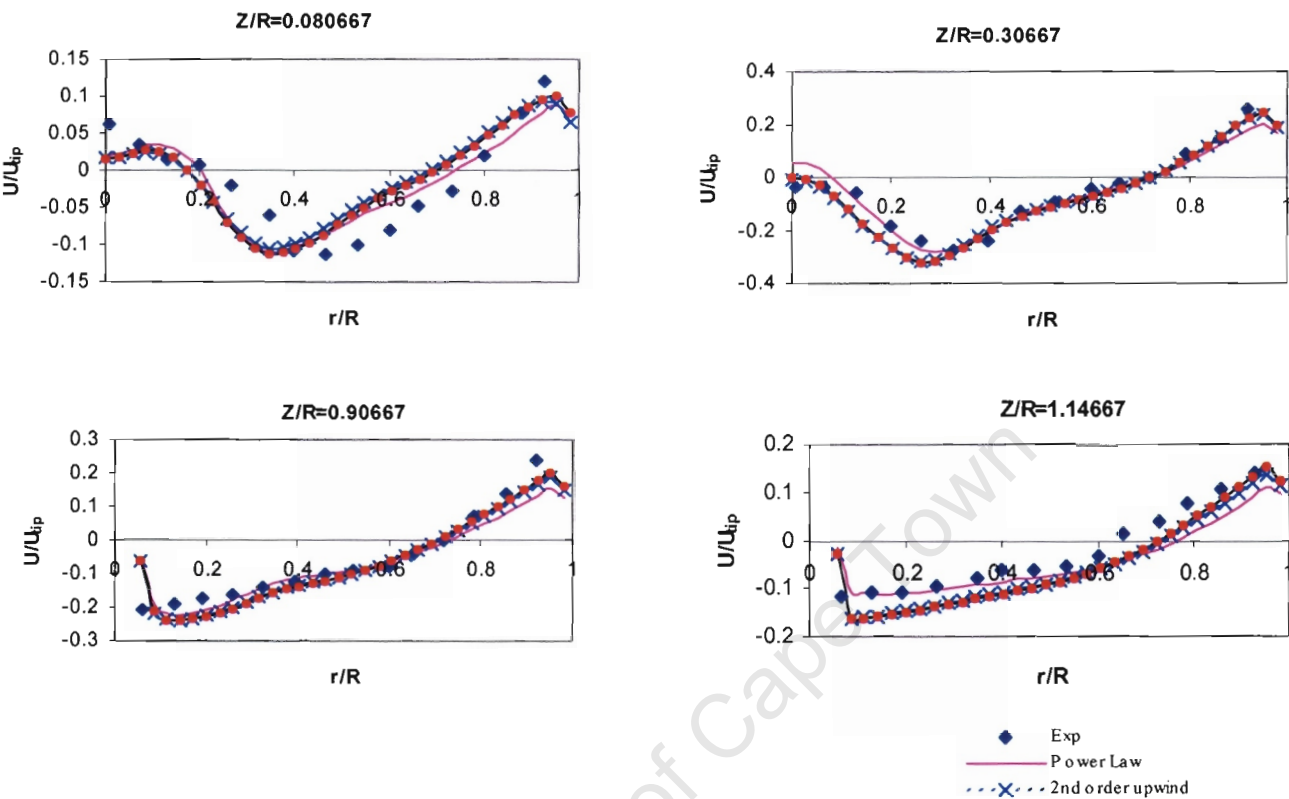


Figure A1: Effect of discretization schemes on the axial velocities:

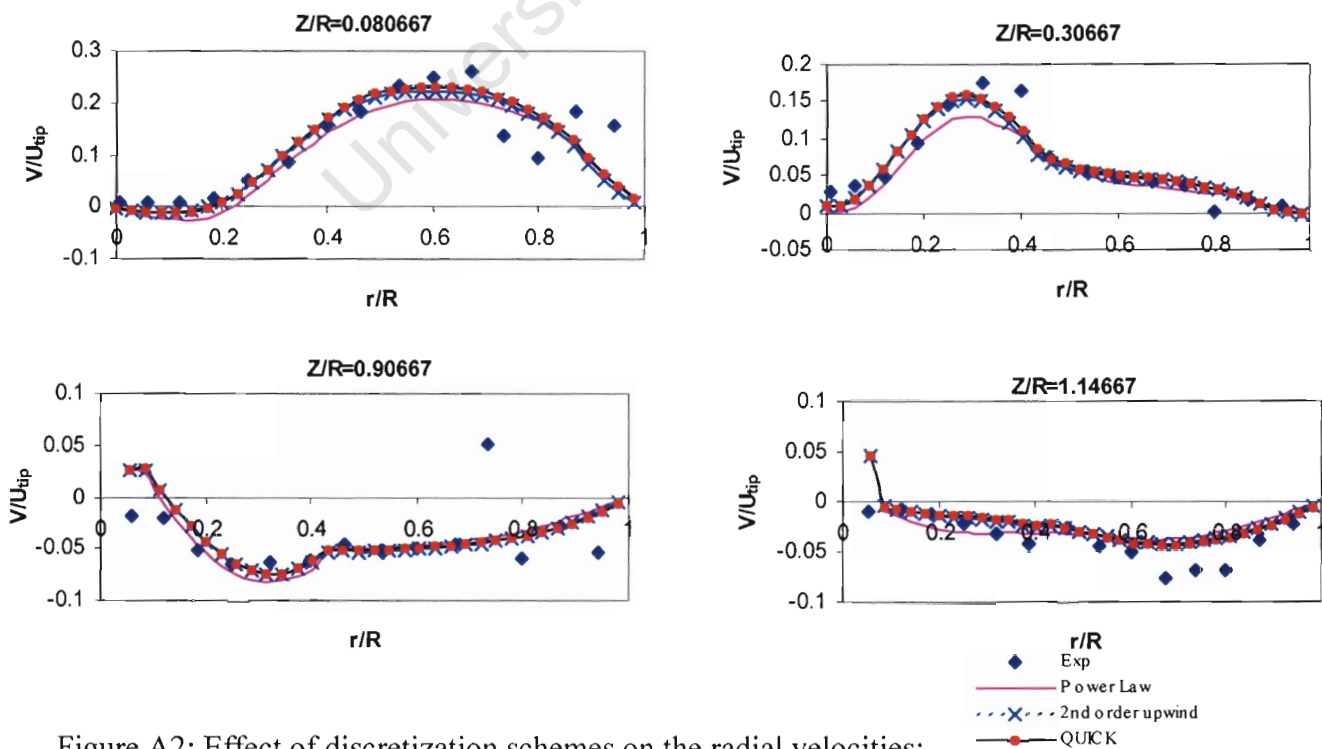


Figure A2: Effect of discretization schemes on the radial velocities:

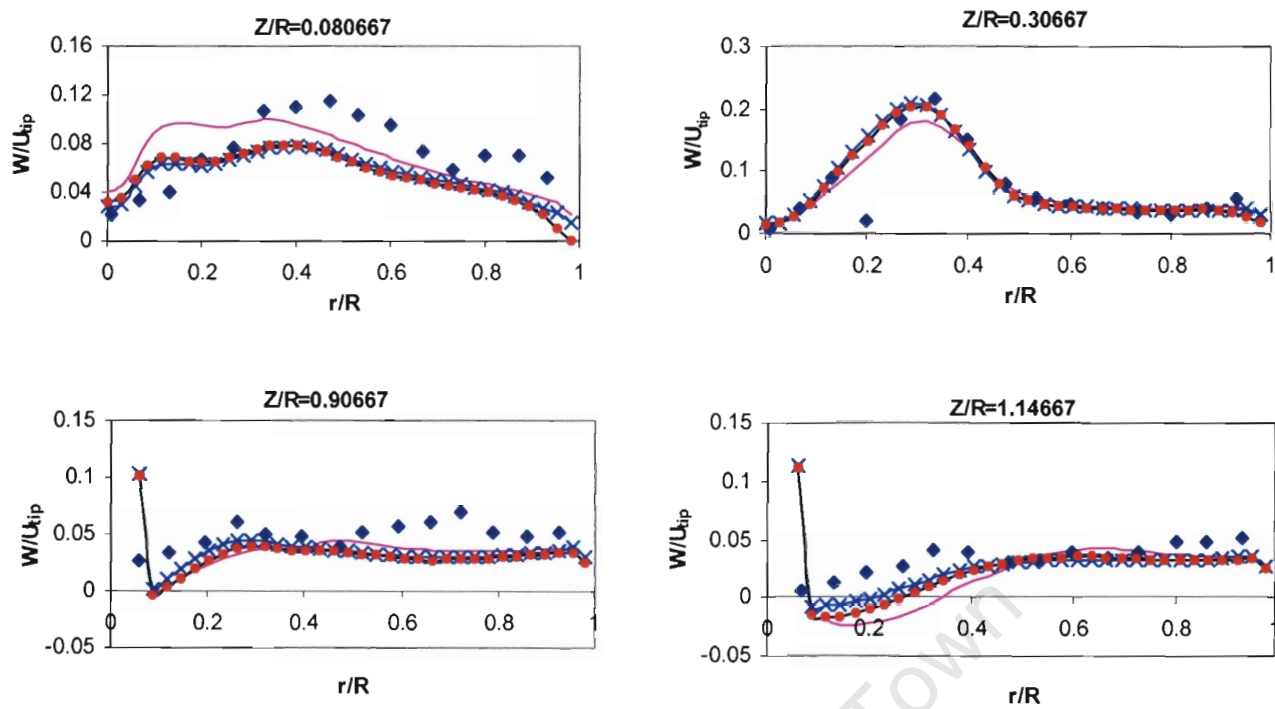


Figure A3: Effect of discretization schemes on the tangential velocities:

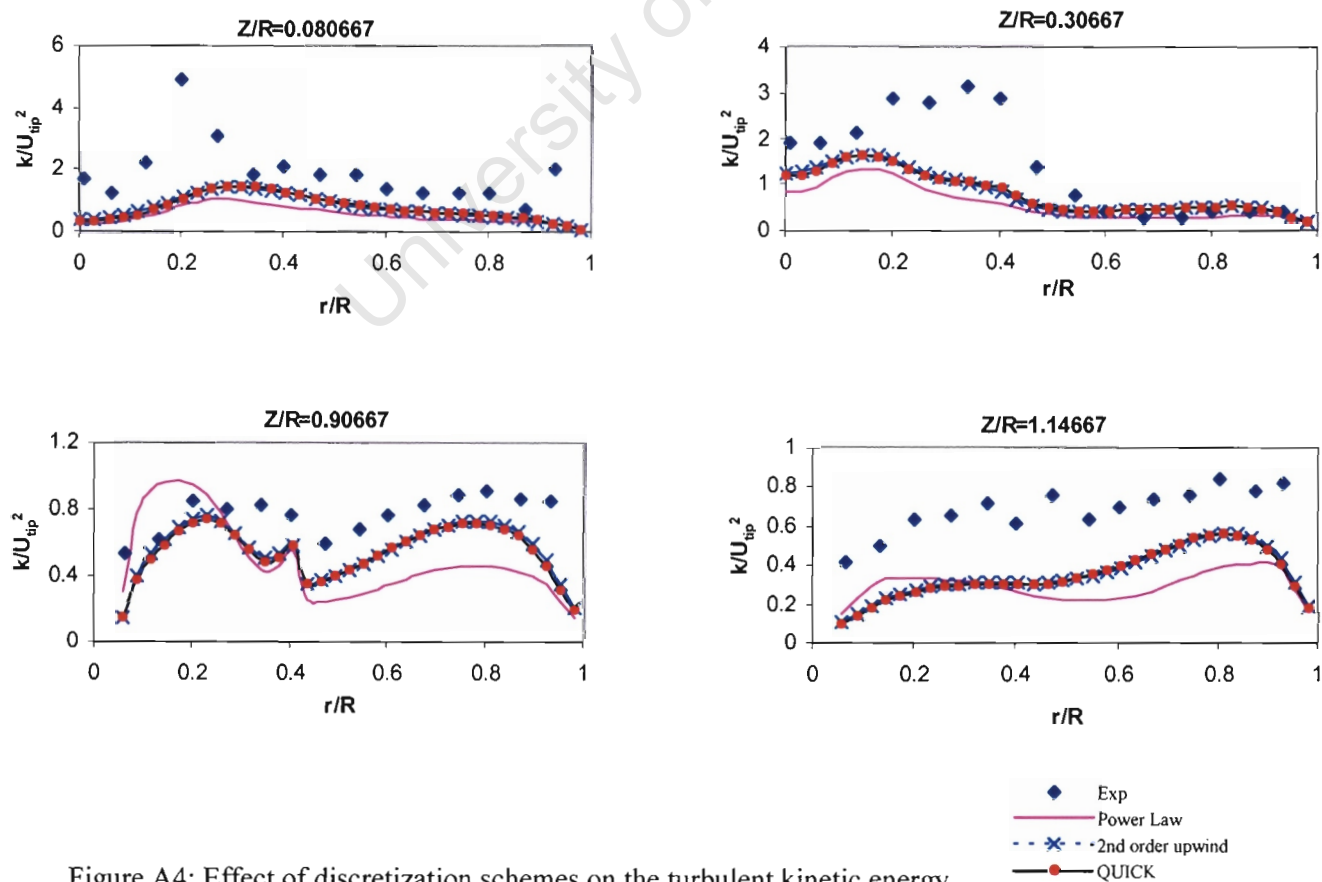


Figure A4: Effect of discretization schemes on the turbulent kinetic energy

Grid independence for 45° pitched blade turbine Stirred tank reactor

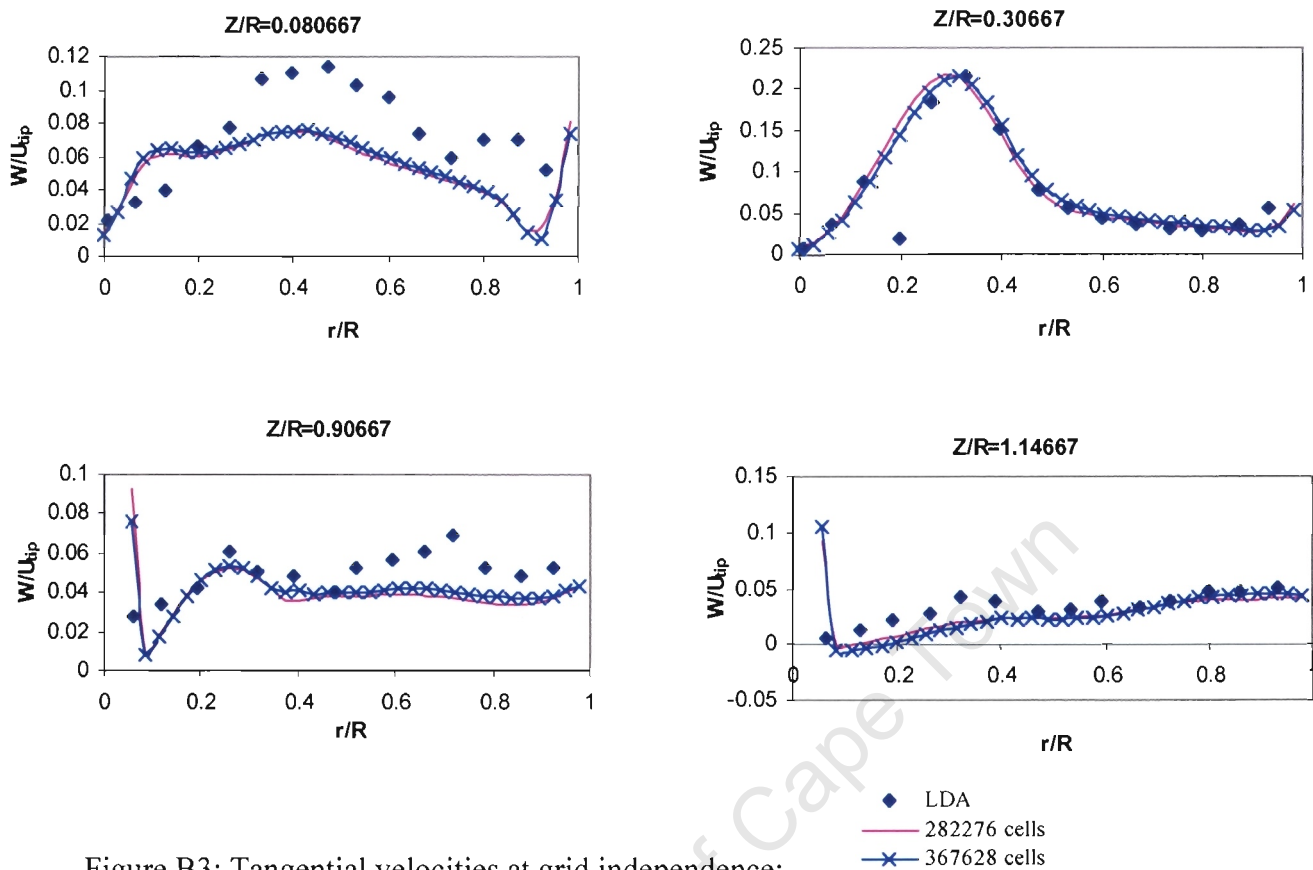


Figure B3: Tangential velocities at grid independence:

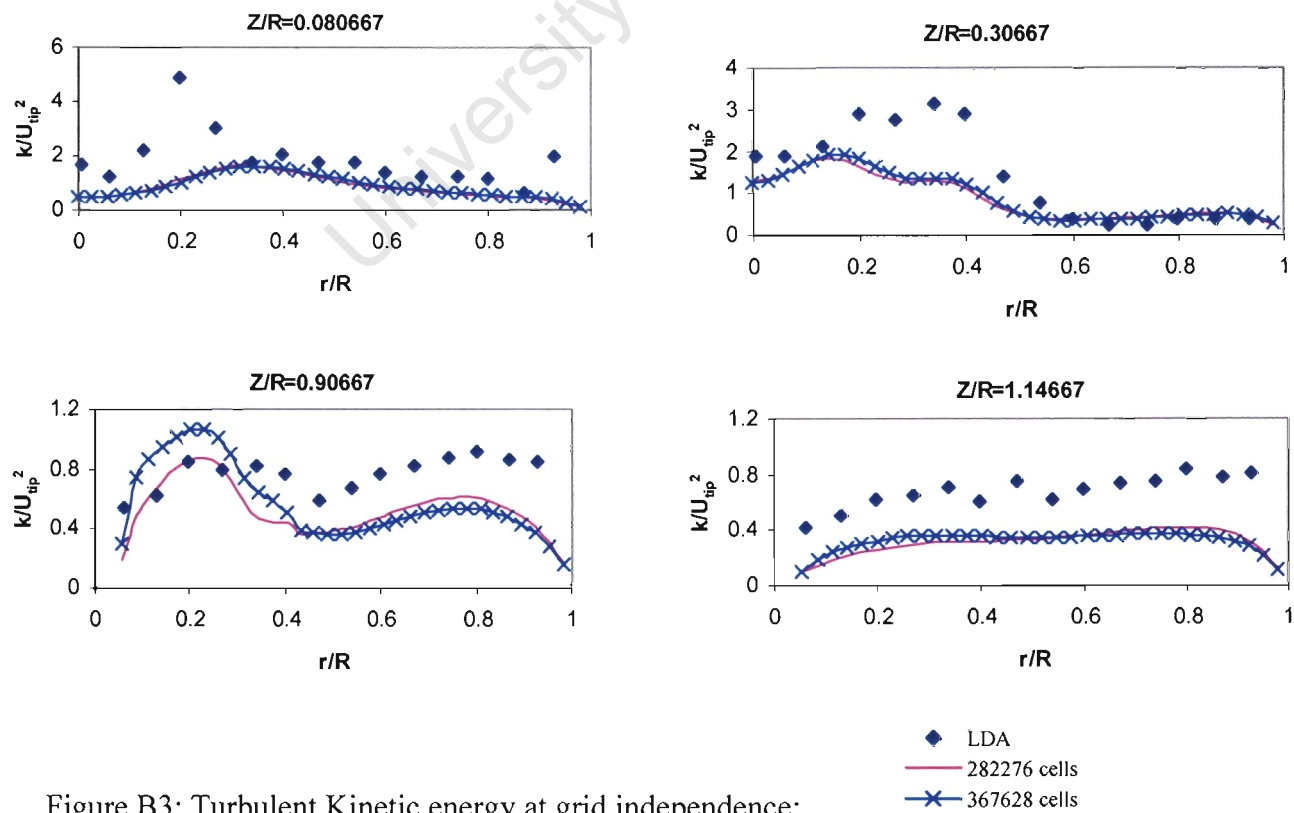


Figure B3: Turbulent Kinetic energy at grid independence:

APPENDIX C

Grid independence for Rushton turbine Stirred tank reactor

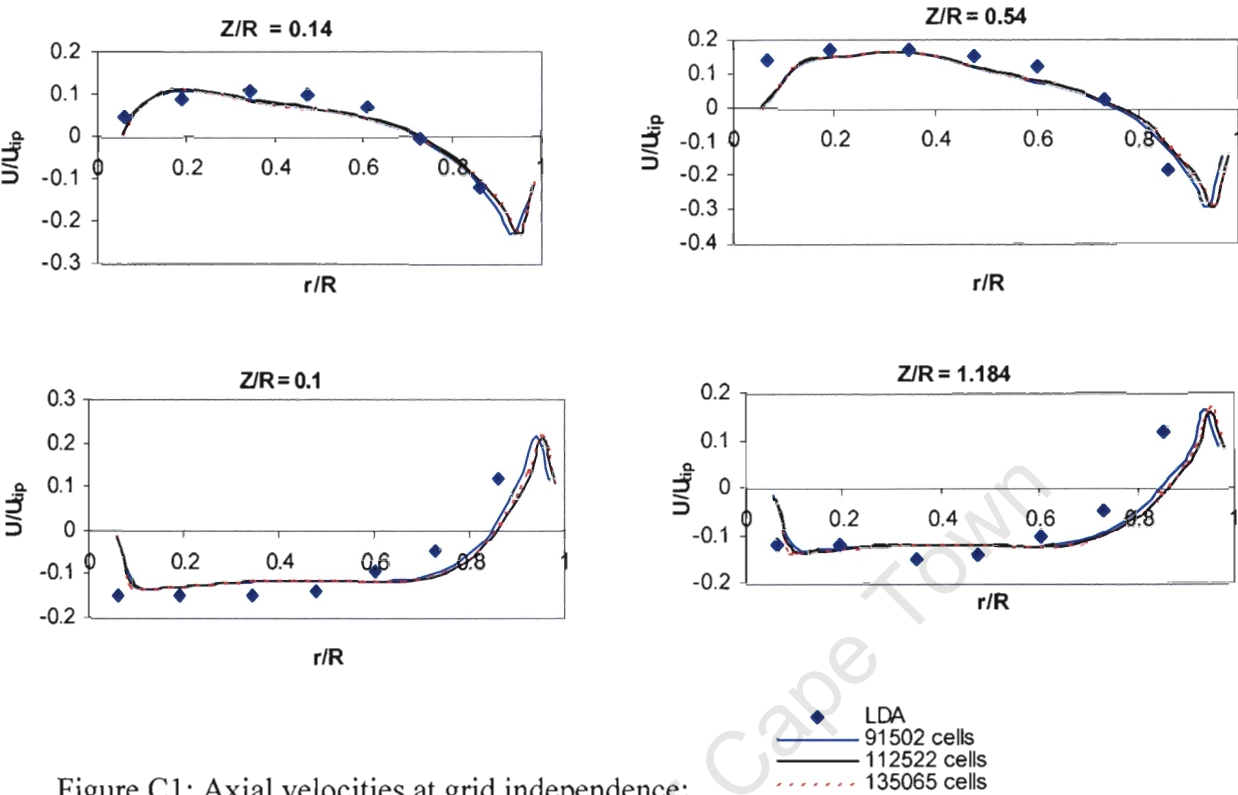


Figure C1: Axial velocities at grid independence:

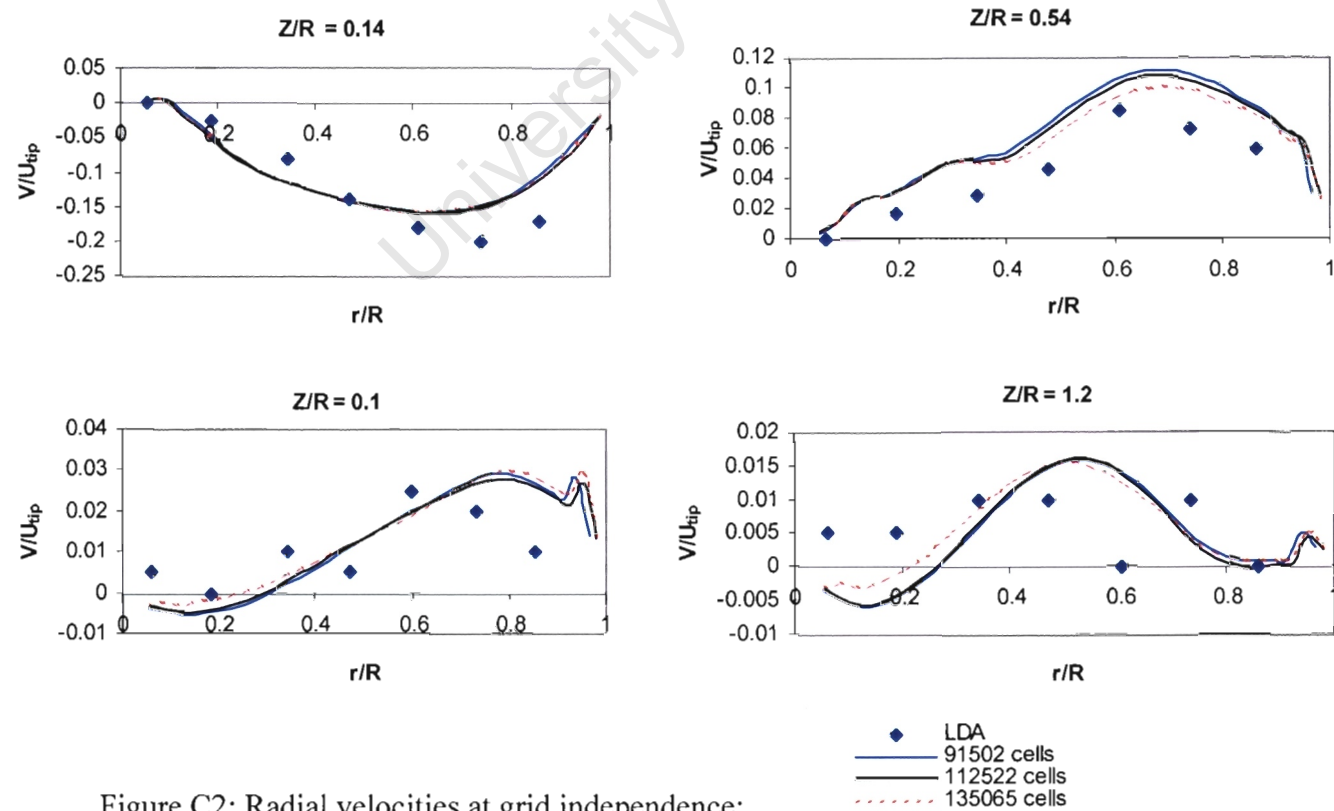


Figure C2: Radial velocities at grid independence:

Grid independence for Rushton turbine Stirred tank reactor

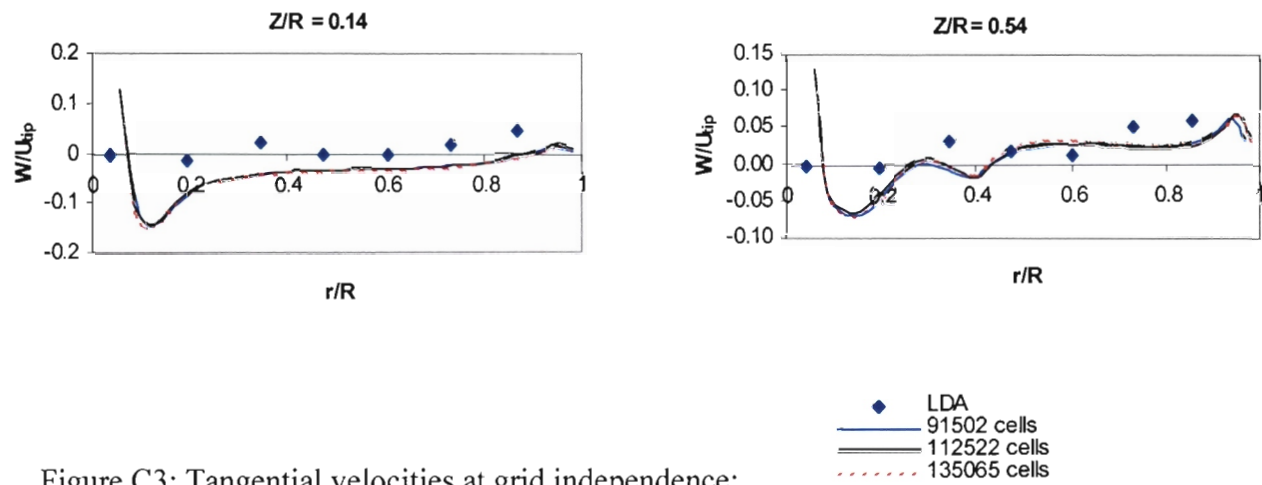


Figure C3: Tangential velocities at grid independence:

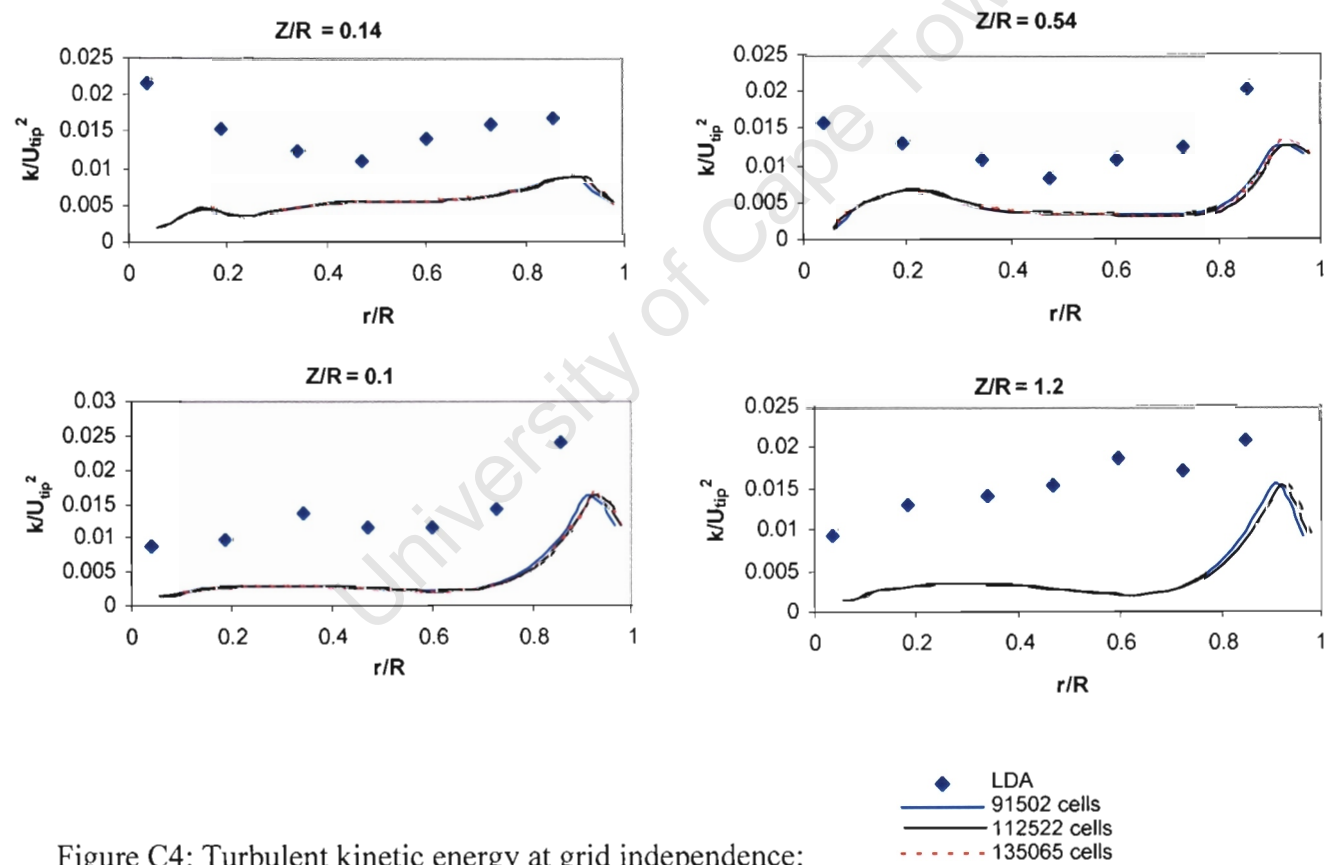


Figure C4: Turbulent kinetic energy at grid independence:

APPENDIX D

Grid independence for 30° pitched blade turbine Stirred tank reactor

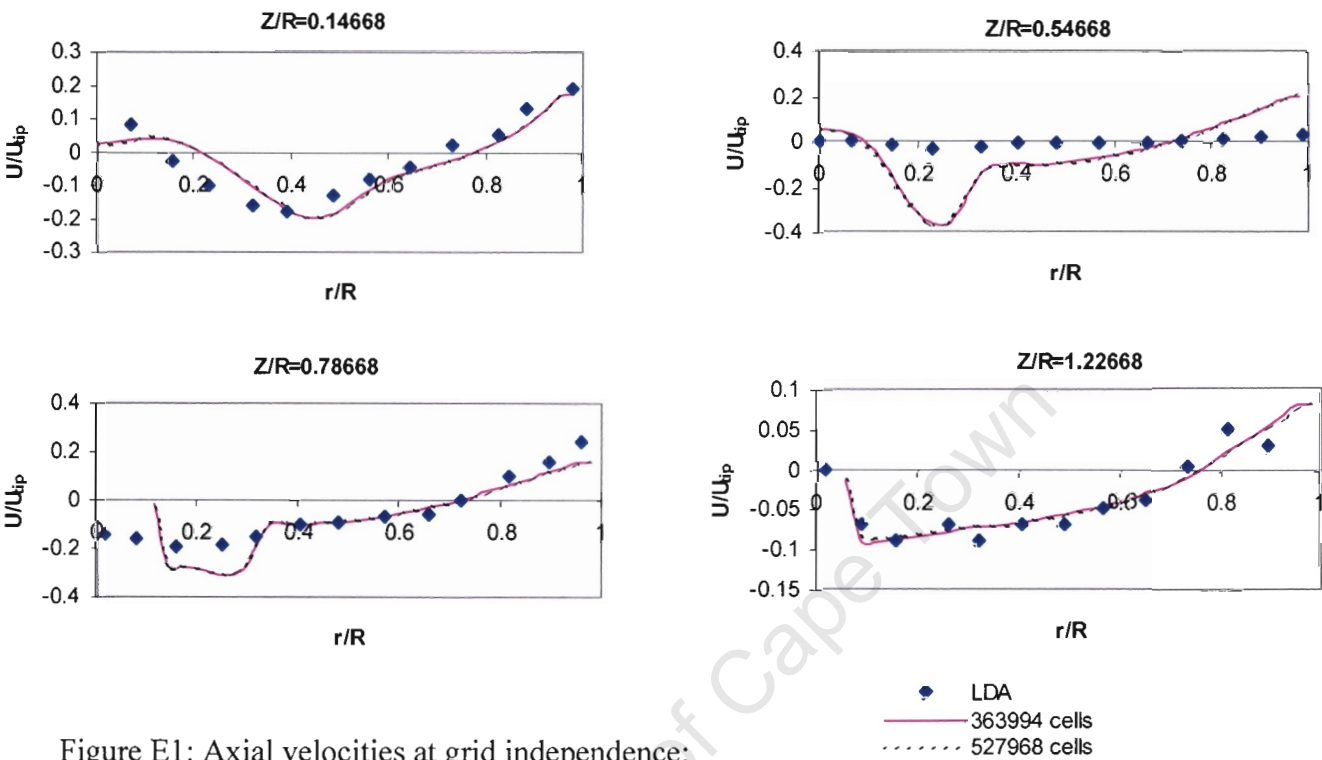


Figure E1: Axial velocities at grid independence:

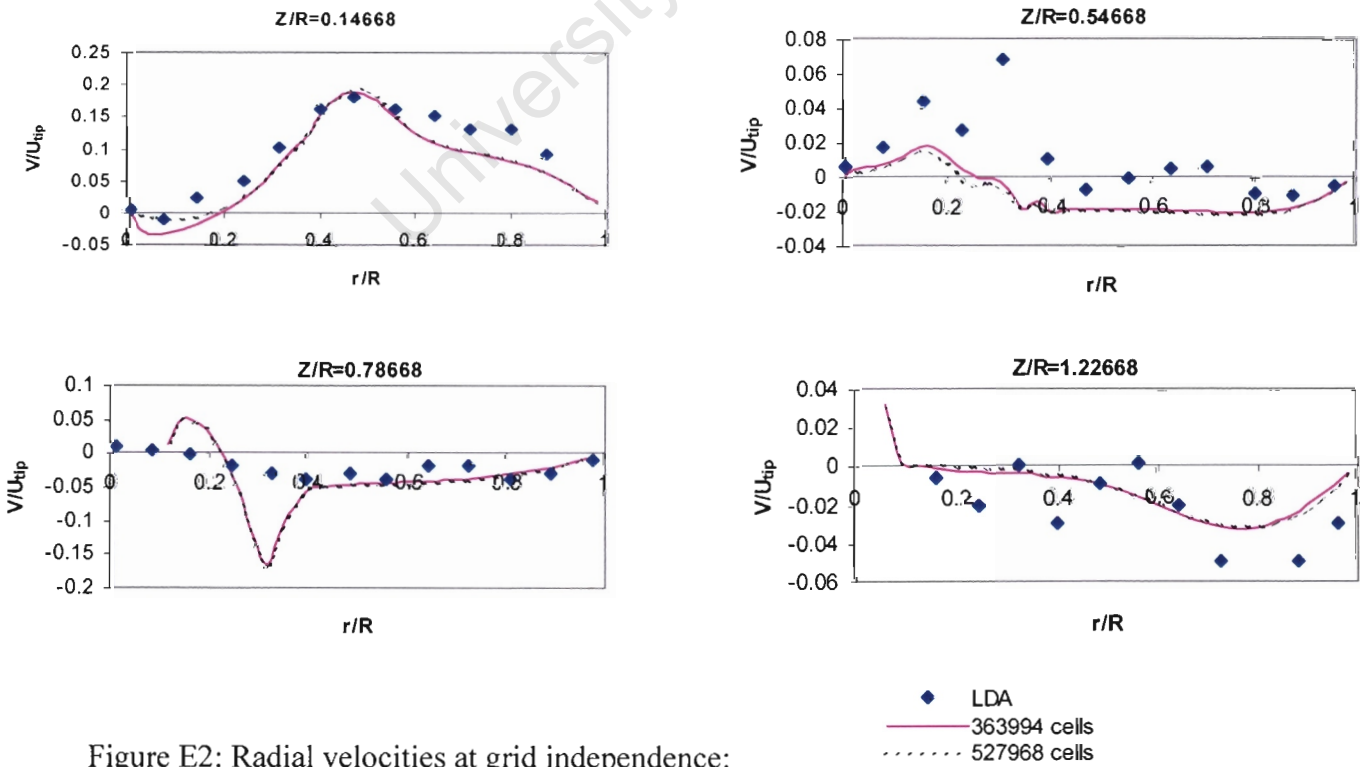


Figure E2: Radial velocities at grid independence:

Grid independence for 30° pitched blade turbine Stirred tank reactor

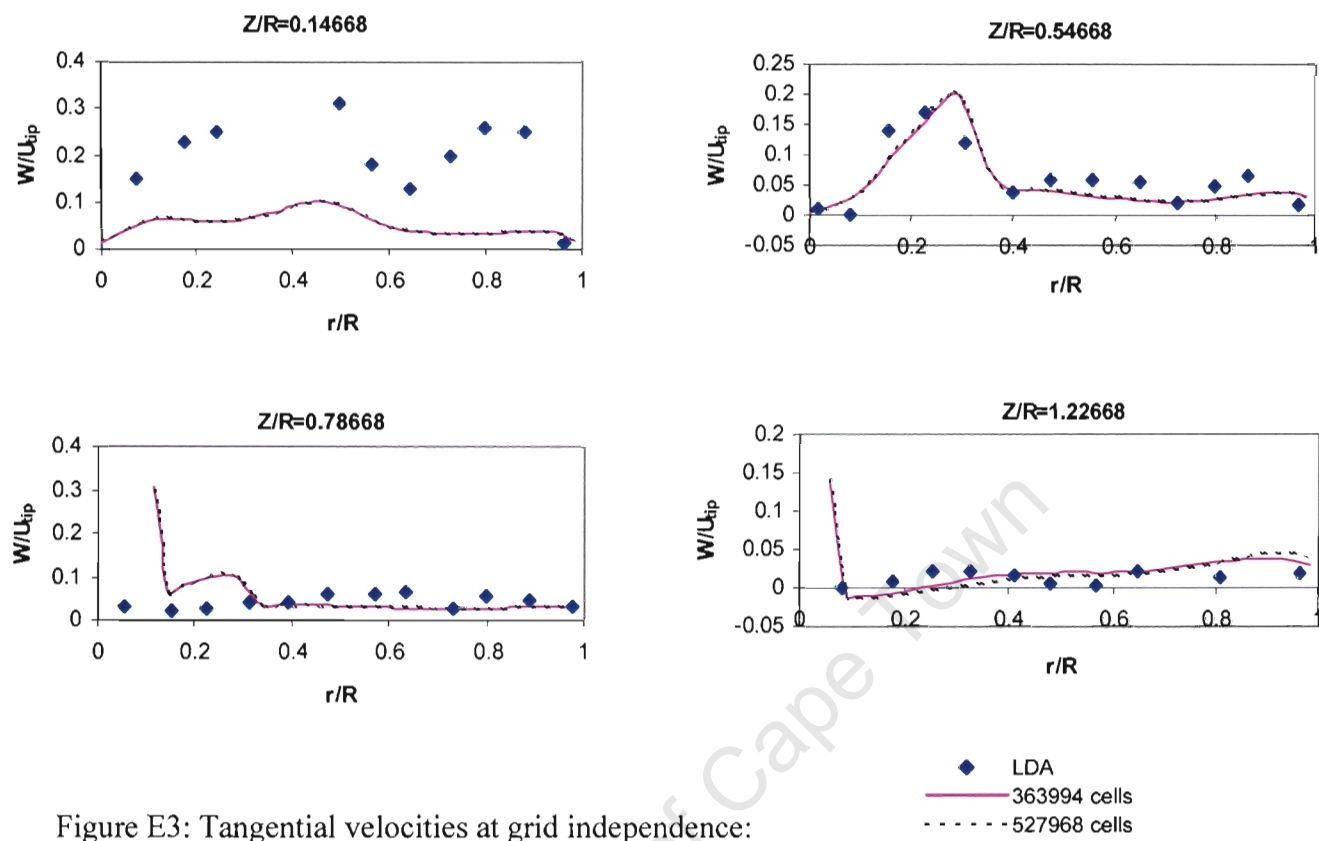


Figure E3: Tangential velocities at grid independence:

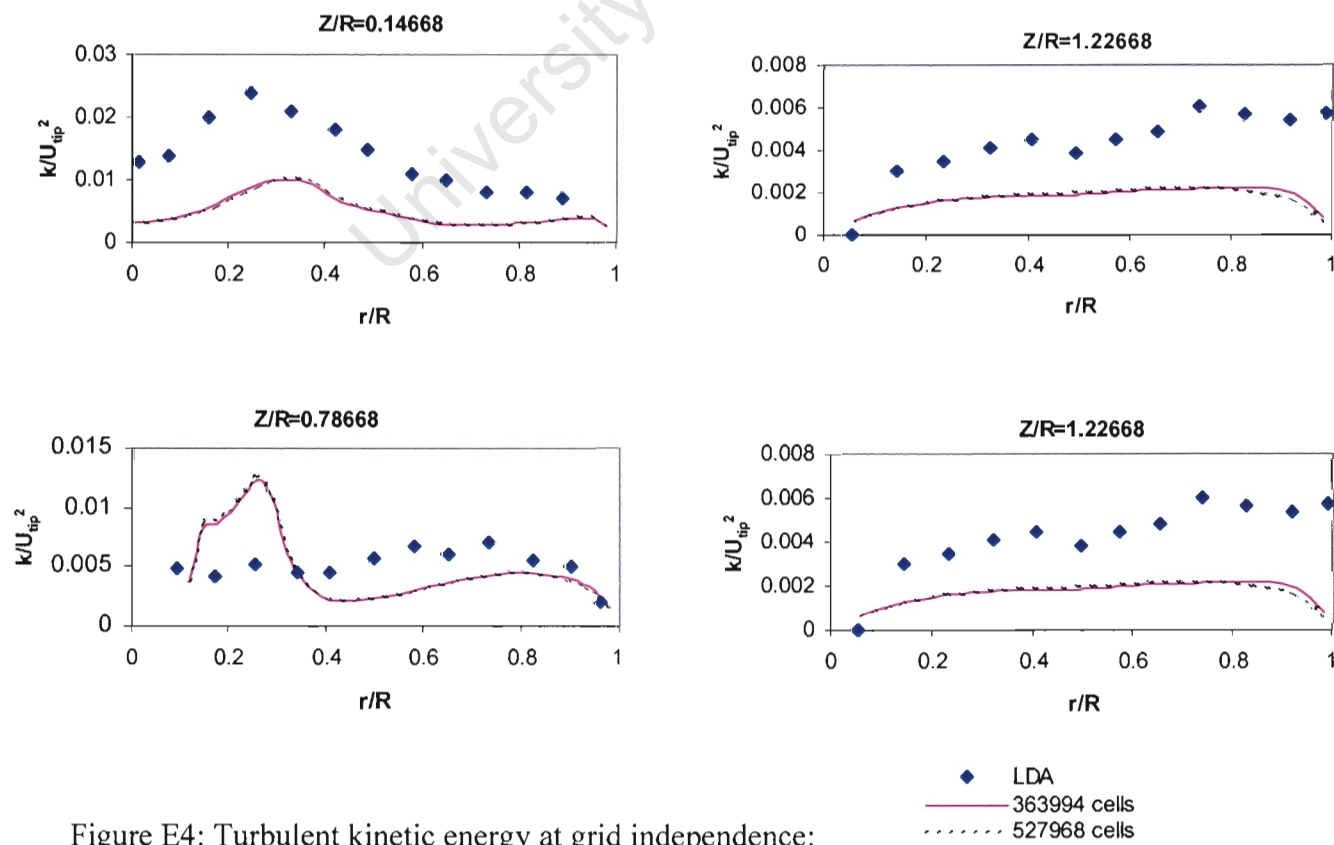


Figure E4: Turbulent kinetic energy at grid independence:

APPENDIX E

Grid independence for 60⁰ pitched blade turbine Stirred tank reactor

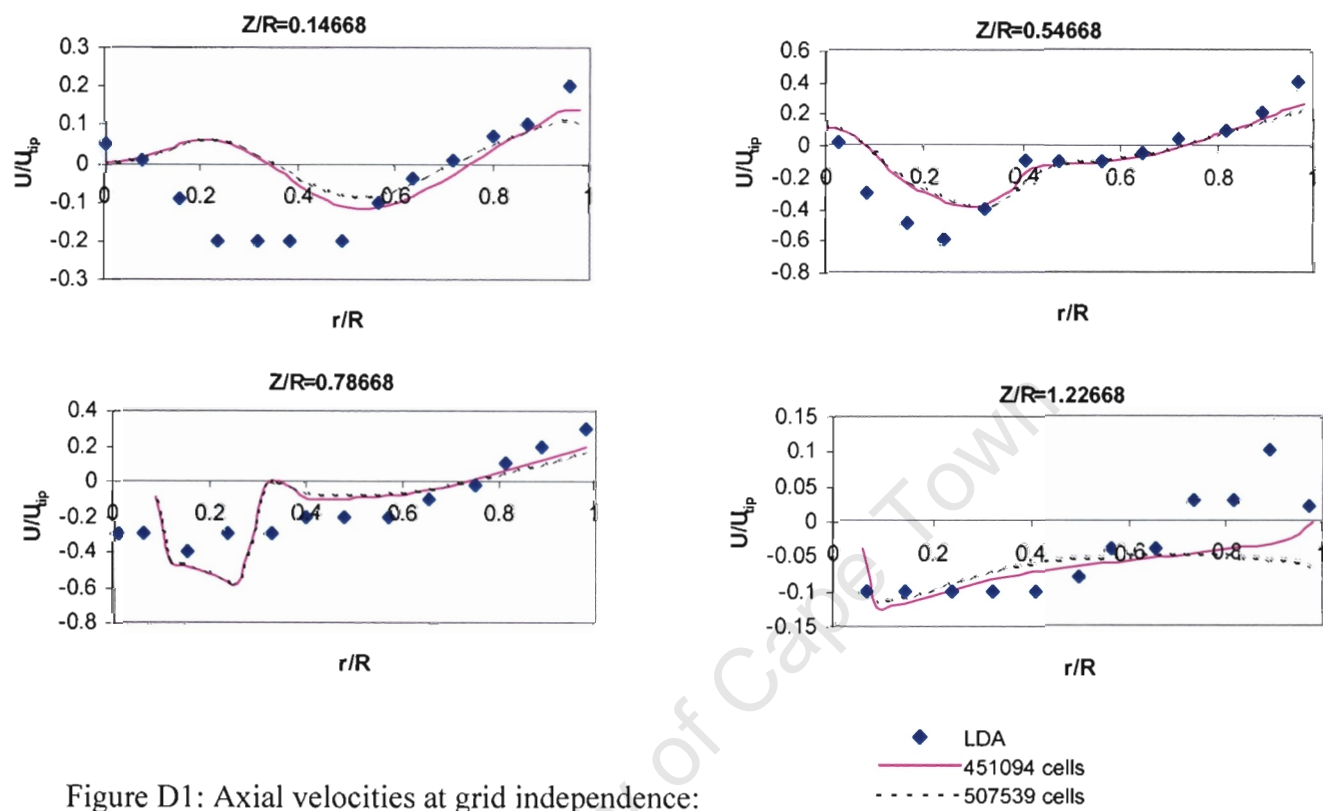


Figure D1: Axial velocities at grid independence:

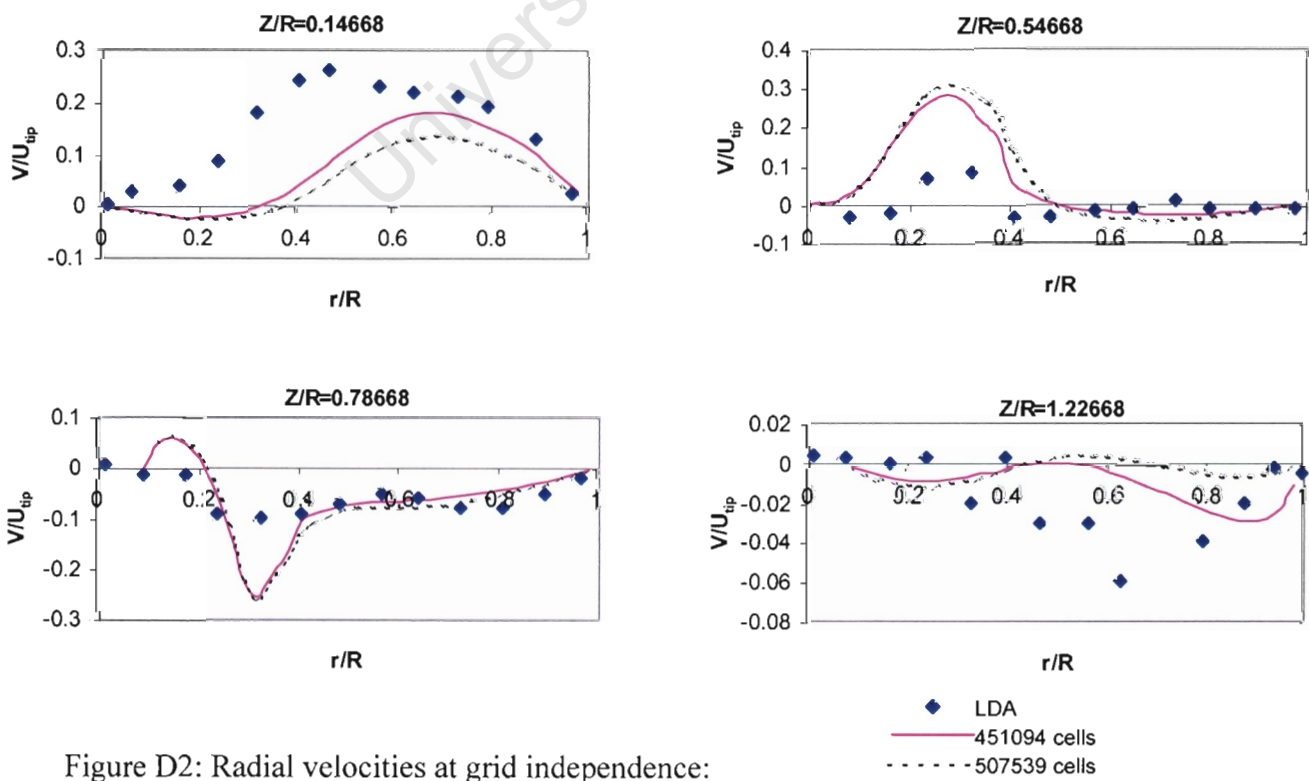


Figure D2: Radial velocities at grid independence:

Grid independence for 60° pitched blade turbine stirred tank reactor

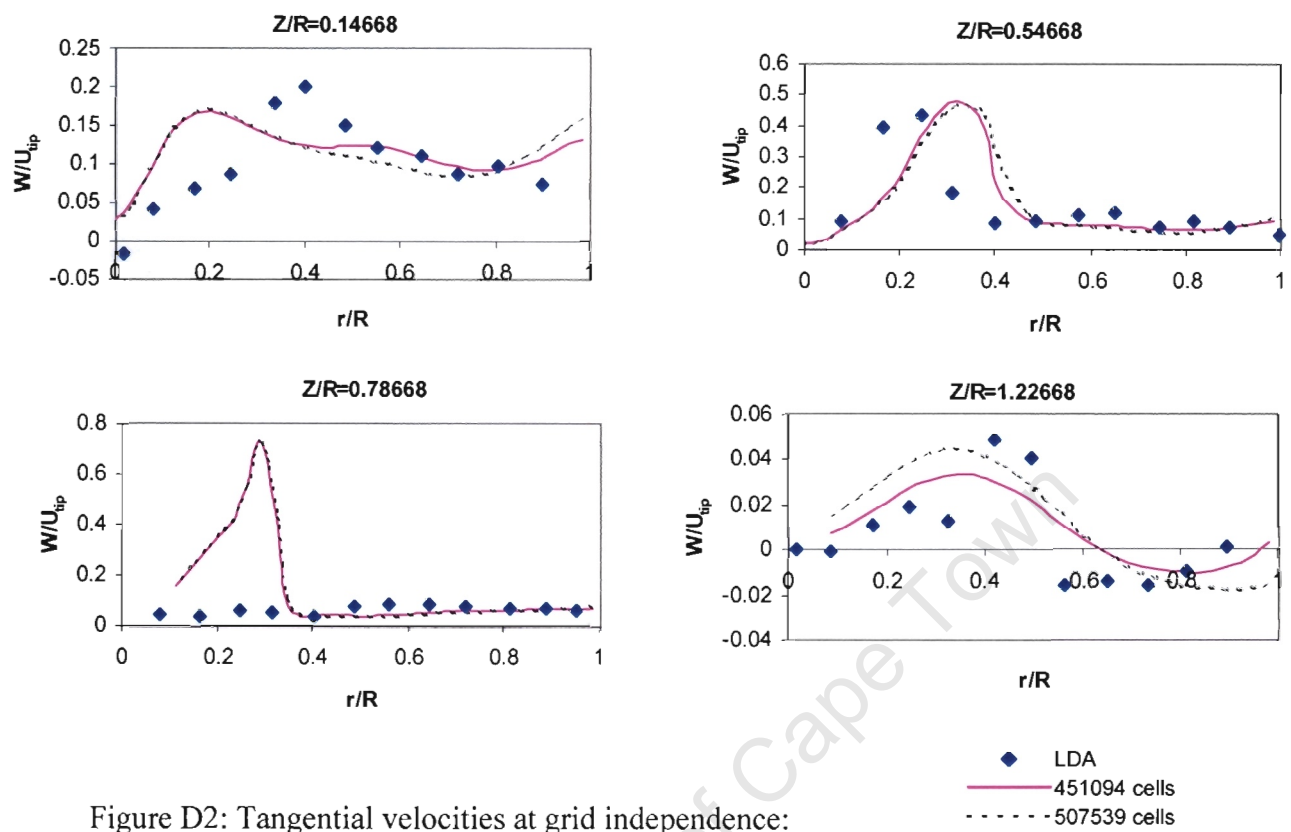


Figure D2: Tangential velocities at grid independence:

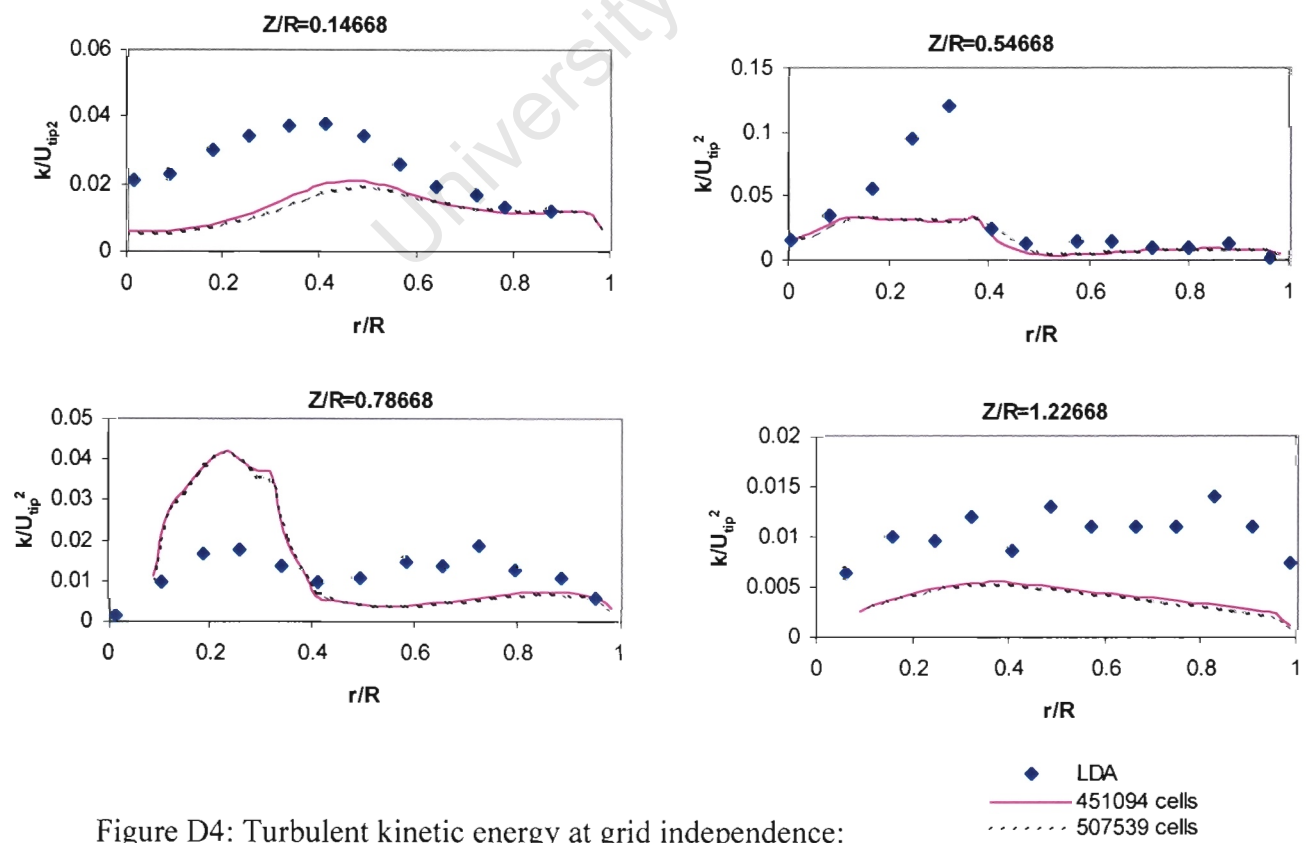


Figure D4: Turbulent kinetic energy at grid independence:

APPENDIX F

Table F1: The parameters combination, error values and Power number for the first set of simulations

C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	u	v	w	k	Total Error	Rank	Power Number(N_p)	Power (Nm/s)	Moment Convergence
0.05	0.9	2.8	0.37006	0.23011	0.20640	0.05478	0.86135	7	2.34	2.92	No
	0.9	2.1	0.27613	0.17411	0.16274	0.03656	0.64953	4	2.26	2.81	No
	0.9	1.4	0.26115	0.15650	0.18080	0.03667	0.63511	2	2.37	2.96	No
	1.25	2.8	0.32797	0.19594	0.18087	0.04256	0.74735	6	2.25	2.81	No
	1.25	2.1	0.22614	0.15178	0.15604	0.03129	0.56525	1	2.25	2.81	Yes
	1.25	1.4	0.45889	0.28941	0.32232	0.05416	1.12478	9	2.43	3.04	No
	1.6	2.8	0.27579	0.16929	0.16271	0.03288	0.64067	3	2.22	2.77	No
	1.6	2.1	0.30839	0.15451	0.19742	0.04130	0.70163	5	2.25	2.81	No
	1.6	1.4	0.35619	0.31028	0.32502	0.07644	1.06793	8	2.61	3.26	No
0.115	0.9	2.8	0.43787	0.28193	0.25954	0.05125	1.03059	8	2.79	3.48	Yes
	0.9	2.1	0.36955	0.23384	0.20993	0.03797	0.85129	6	2.43	3.03	Yes
	0.9	1.4	0.21954	0.15441	0.15522	0.04443	0.57361	1	2.34	2.91	No
	1.25	2.8	0.41724	0.26248	0.24062	0.04056	0.96090	7	2.47	3.08	Yes
	1.25	2.1	0.30213	0.18235	0.17050	0.03648	0.69147	3	2.26	2.82	No
	1.25	1.4	0.35399	0.21426	0.31627	0.05661	0.94113	5	2.56	3.20	No
	1.6	2.8	0.36885	0.22183	0.20474	0.03495	0.83037	4	2.29	2.86	Yes
	1.6	2.1	0.22961	0.14470	0.16405	0.04444	0.58280	2	2.27	2.83	Yes
	1.6	1.4	0.60038	0.36104	0.45561	0.07741	1.49445	9	2.48	3.10	No
0.18	0.9	2.8	0.45367	0.29518	0.28034	0.05359	1.08277	8	3.31	4.13	Yes
	0.9	2.1	0.34094	0.21243	0.19289	0.03762	0.78388	4	2.36	2.95	No
	0.9	1.4	0.25371	0.16696	0.15880	0.04786	0.62733	2	2.37	2.96	No
	1.25	2.8	0.44482	0.28534	0.26592	0.03997	1.03605	7	2.77	3.45	Yes
	1.25	2.1	0.35170	0.21590	0.19815	0.03826	0.80400	5	2.35	2.93	No
	1.25	1.4	0.30719	0.19439	0.23031	0.06010	0.79199	3	2.41	3.01	No
	1.6	2.8	0.41640	0.25896	0.24026	0.03544	0.95105	6	2.40	3.00	No
	1.6	2.1	0.24953	0.16030	0.15649	0.04714	0.61346	1	2.22	2.77	No
	1.6	1.4	0.43778	0.30404	0.37349	0.07780	1.19311	9	2.60	3.24	No

Table F2: The parameters combination, error values and Power number for the second set of simulations

C_{μ}	$C_{\epsilon 1}$	$C_{\epsilon 2}$	u	v	w	k	Total Error	Rank	Power Number(N_p)	Power (Nm/s)	Moment Convergence
0.03	1	2.6	0.27946	0.17410	0.16378	0.04551	0.66285	8	2.22	2.77	No
	1	2.2	0.23127	0.15610	0.15477	0.03322	0.57537	2	2.24	2.80	No
	1	1.8	0.24666	0.14653	0.16597	0.02771	0.58687	4	2.29	2.85	No
	1.2	2.6	0.25597	0.16507	0.15893	0.03747	0.61744	6	2.22	2.77	No
	1.2	2.2	0.22368	0.14559	0.16229	0.02779	0.55934	1	2.28	2.84	No
	1.2	1.8	0.27484	0.15640	0.18719	0.03232	0.65076	7	2.32	2.89	No
	1.4	2.6	0.23195	0.15619	0.15994	0.03061	0.57869	3	2.25	2.80	No
	1.4	2.2	0.25550	0.15186	0.17297	0.02865	0.60898	5	2.29	2.85	No
	1.4	1.8	0.41152	0.20762	0.23797	0.03654	0.89365	9	2.53	3.16	No
0.065	1	2.6	0.36520	0.22652	0.20395	0.04533	0.84100	9	2.34	2.92	No
	1	2.2	0.30562	0.18741	0.17313	0.03672	0.70289	7	2.27	2.84	No
	1	1.8	0.23353	0.15792	0.15290	0.03418	0.57854	2	2.26	2.82	No
	1.2	2.6	0.33781	0.20383	0.18681	0.03952	0.76797	8	2.28	2.84	No
	1.2	2.2	0.27255	0.16987	0.16086	0.03367	0.63695	4	2.23	2.78	No
	1.2	1.8	0.22737	0.14165	0.16234	0.03623	0.56760	1	2.29	2.86	Yes
	1.4	2.6	0.30682	0.18205	0.17107	0.03478	0.69472	6	2.23	2.78	Yes
	1.4	2.2	0.23646	0.15691	0.15632	0.03370	0.58338	3	2.23	2.79	No
	1.4	1.8	0.28442	0.14596	0.19301	0.04531	0.66870	5	2.31	2.89	No
0.1	1	2.6	0.40964	0.25944	0.23483	0.04369	0.94760	9	3.11	3.11	Yes
	1	2.2	0.35459	0.22082	0.19988	0.03739	0.81268	7	2.95	2.95	No
	1	1.8	0.27185	0.17173	0.16159	0.03694	0.64211	3	2.85	2.85	No
	1.2	2.6	0.38695	0.24079	0.21825	0.03911	0.88509	8	2.96	2.96	No
	1.2	2.2	0.31858	0.19222	0.17813	0.03525	0.72418	5	2.84	2.84	No
	1.2	1.8	0.22966	0.15537	0.15310	0.04019	0.57833	1	2.81	2.81	No
	1.4	2.6	0.35516	0.21403	0.19674	0.03565	0.80159	6	2.86	2.86	No
	1.4	2.2	0.27631	0.16955	0.16122	0.03636	0.64345	4	2.77	2.77	No
	1.4	1.8	0.26594	0.14768	0.17148	0.04678	0.63189	2	2.82	2.82	Yes

Table F3: The parameters combination, error values and Power number for the third set of simulations

C_μ	$C_{\varepsilon 1}$	$C_{\varepsilon 2}$	u	v	w	k	Total Error	Rank	Power Number(N_p)	Power (Nm/s)	Moment Convergence
0.045	1.1	2.4	0.28284	0.17476	0.16420	0.03741	0.65921	9	2.23	2.78	No
	1.1	2.2	0.25324	0.16405	0.15690	0.03334	0.60753	6	2.23	2.78	No
	1.1	2	0.22428	0.15196	0.15437	0.03081	0.56142	1	2.26	2.82	No
	1.25	2.4	0.26123	0.16594	0.15888	0.03342	0.61948	8	2.04	2.55	No
	1.25	2.2	0.23168	0.15530	0.15583	0.03078	0.57360	4	2.24	2.80	No
	1.25	2	0.22800	0.14389	0.16358	0.03083	0.56630	2	2.40	0.30	Yes
	1.4	2.4	0.23835	0.15836	0.15762	0.03082	0.58515	5	2.23	2.79	No
	1.4	2.2	0.22737	0.14479	0.16497	0.03052	0.56765	3	2.28	2.84	Yes
	1.4	2	0.27006	0.15047	0.17436	0.03541	0.63030	7	2.27	2.84	No
0.07	1.1	2.4	0.33115	0.20132	0.18432	0.03817	0.75495	9	2.29	2.85	No
	1.1	2.2	0.29754	0.18176	0.16927	0.03510	0.68366	7	2.25	2.81	No
	1.1	2	0.26012	0.16634	0.15776	0.03409	0.61831	4	2.24	2.80	No
	1.25	2.4	0.30724	0.18448	0.17204	0.03507	0.69883	8	2.24	2.80	No
	1.25	2.2	0.27101	0.16890	0.16033	0.03373	0.63398	5	2.23	2.78	No
	1.25	2	0.23299	0.15591	0.15435	0.03478	0.57803	2	2.24	2.79	No
	1.4	2.4	0.28033	0.17102	0.16264	0.03343	0.64742	6	2.22	2.77	No
	1.4	2.2	0.24250	0.15931	0.15625	0.03427	0.59233	3	2.23	2.78	No
	1.4	2	0.22925	0.14343	0.16457	0.03738	0.57463	1	2.27	2.84	Yes
0.095	1.1	2.4	0.36627	0.22731	0.20556	0.03827	0.83742	9	2.35	2.94	No
	1.1	2.2	0.29754	0.18176	0.16927	0.03510	0.68366	5	2.25	2.81	No
	1.1	2	0.29081	0.17879	0.16719	0.03554	0.67234	4	2.27	2.83	No
	1.25	2.4	0.34125	0.20629	0.18951	0.03576	0.77281	8	2.29	2.86	No
	1.25	2.2	0.30321	0.18269	0.17072	0.03500	0.69162	6	2.25	2.81	No
	1.25	2	0.25948	0.16525	0.15737	0.03696	0.61906	2	2.23	2.78	No
	1.4	2.4	0.31348	0.18568	0.17391	0.03454	0.70762	7	2.24	2.80	No
	1.4	2.2	0.27109	0.16778	0.15999	0.03611	0.63497	3	2.22	2.77	No
	1.4	2	0.22795	0.15187	0.15589	0.03981	0.57553	1	2.25	2.80	Yes

Table F4: The parameters combination, error values and Power number for the fourth set of simulations

C_{μ}	$C_{\epsilon 1}$	$C_{\epsilon 2}$	u	v	w	k	Total Error	Rank	Power Number(N_p)	Power (Nm/s)	Moment Convergence
0.045	1.22	2.15	0.22901	0.15396	0.15559	0.03070	0.56925	2	2.24	2.80	No
	1.22	1.95	0.23115	0.14260	0.16460	0.03099	0.56934	3	2.29	2.85	Yes
	1.22	1.75	0.28653	0.15645	0.18279	0.03702	0.66279	7	2.24	2.80	No
	1.31	2.15	0.22407	0.14694	0.16020	0.03023	0.56144	1	2.27	2.83	Yes
	1.31	1.95	0.25611	0.14804	0.16970	0.03346	0.60731	5	2.27	2.83	Yes
	1.31	1.75	0.29814	0.14593	0.24185	0.03668	0.72259	8	2.41	3.01	No
	1.39	2.15	0.23056	0.14467	0.16671	0.03099	0.57293	4	2.28	2.84	Yes
	1.39	1.95	0.28809	0.14817	0.17772	0.03669	0.65067	6	2.27	2.84	No
	1.39	1.75	0.35940	0.19410	0.25094	0.04096	0.84540	9	2.37	2.96	No
0.0675	1.22	2.15	0.26352	0.16656	0.15858	0.03360	0.62226	7	2.23	2.78	No
	1.22	1.95	0.22691	0.15300	0.15425	0.03470	0.56885	2	2.25	2.81	No
	1.22	1.75	0.24577	0.14317	0.16660	0.03846	0.59400	4	2.29	2.86	Yes
	1.31	2.15	0.24707	0.16110	0.15603	0.03373	0.59793	6	2.22	2.78	No
	1.31	1.95	0.22416	0.14407	0.16041	0.03593	0.56456	1	2.27	2.84	Yes
	1.31	1.75	0.28755	0.15287	0.17751	0.04285	0.66078	8	2.26	2.82	Yes
	1.39	2.15	0.23263	0.15497	0.15622	0.03438	0.57819	3	2.24	2.79	No
	1.39	1.95	0.24421	0.14349	0.16845	0.03825	0.59439	5	2.28	2.85	No
	1.39	1.75	0.34542	0.17868	0.19817	0.04556	0.76783	9	2.33	2.91	No
0.09	1.22	2.15	0.29299	0.17816	0.16703	0.03493	0.67311	9	2.25	2.80	No
	1.22	1.95	0.24995	0.16252	0.15557	0.03697	0.60501	5	2.23	2.79	No
	1.22	1.75	0.22047	0.14344	0.15852	0.04068	0.56311	1	2.28	2.85	Yes
	1.31	2.15	0.27435	0.16963	0.16093	0.03540	0.64030	7	2.23	2.78	No
	1.31	1.95	0.23112	0.15476	0.15431	0.03849	0.57868	3	2.24	2.79	No
	1.31	1.75	0.25399	0.14438	0.16841	0.04381	0.61060	4	2.28	2.85	No
	1.39	2.15	0.25708	0.16375	0.15729	0.03643	0.61455	6	2.22	2.77	No
	1.39	1.95	0.22472	0.14499	0.15981	0.04021	0.56972	2	2.27	2.83	Yes
	1.39	1.75	0.28638	0.15988	0.19550	0.04819	0.68995	8	2.22	2.77	No

APPENDIX G

Performance of the optimum turbulence model parameters in 45° Pitched blade turbine

$$C_{\mu}=0.045, C_{\epsilon 1}=1.22, C_{\epsilon 2}=1.95$$

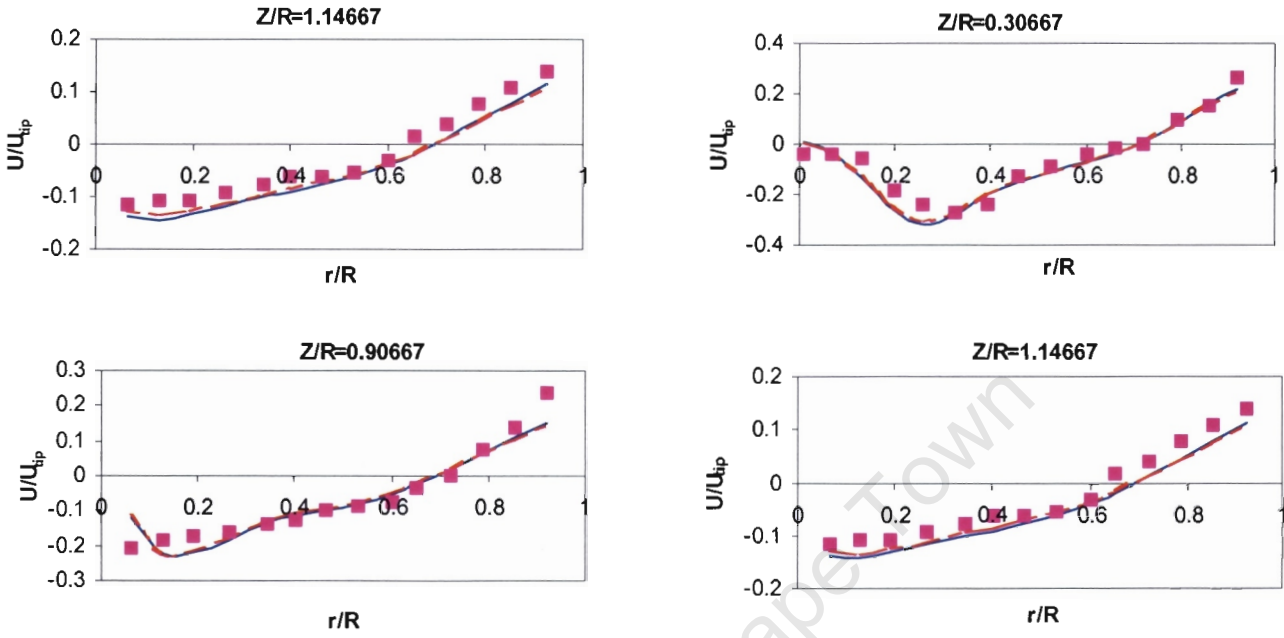


Figure G1: Axial velocities of 45° pitched blade turbine with model parameters $C_{\mu}=0.045$, $C_{\epsilon 1}=1.22$, $C_{\epsilon 2}=1.95$: ■ LDA, — Standard $k-\epsilon$ model, - - - Optimum model parameters

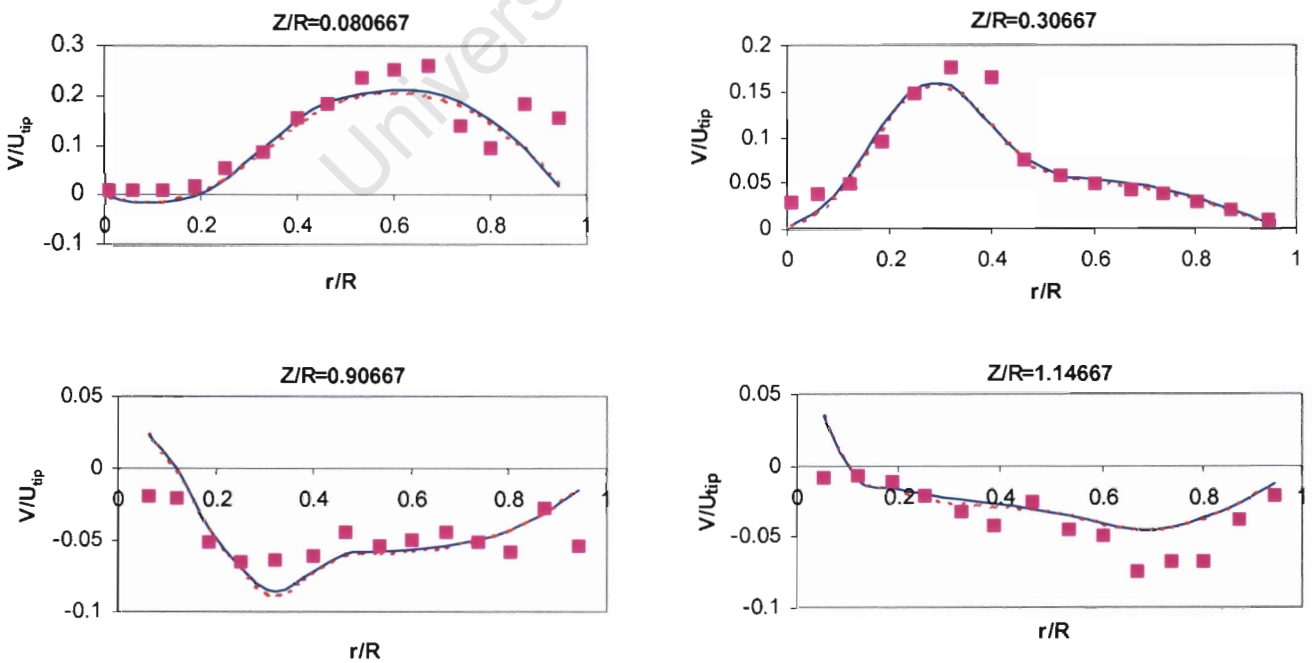


Figure G2: Radial velocities of 45° pitched blade turbine with model parameters $C_{\mu}=0.045$, $C_{\epsilon 1}=1.22$, $C_{\epsilon 2}=1.95$: ■ LDA, — Standard $k-\epsilon$ model, - - - Optimum model parameters

$C_\mu=0.045$, $C_{\epsilon 1}=1.22$, $C_{\epsilon 2}=1.95$

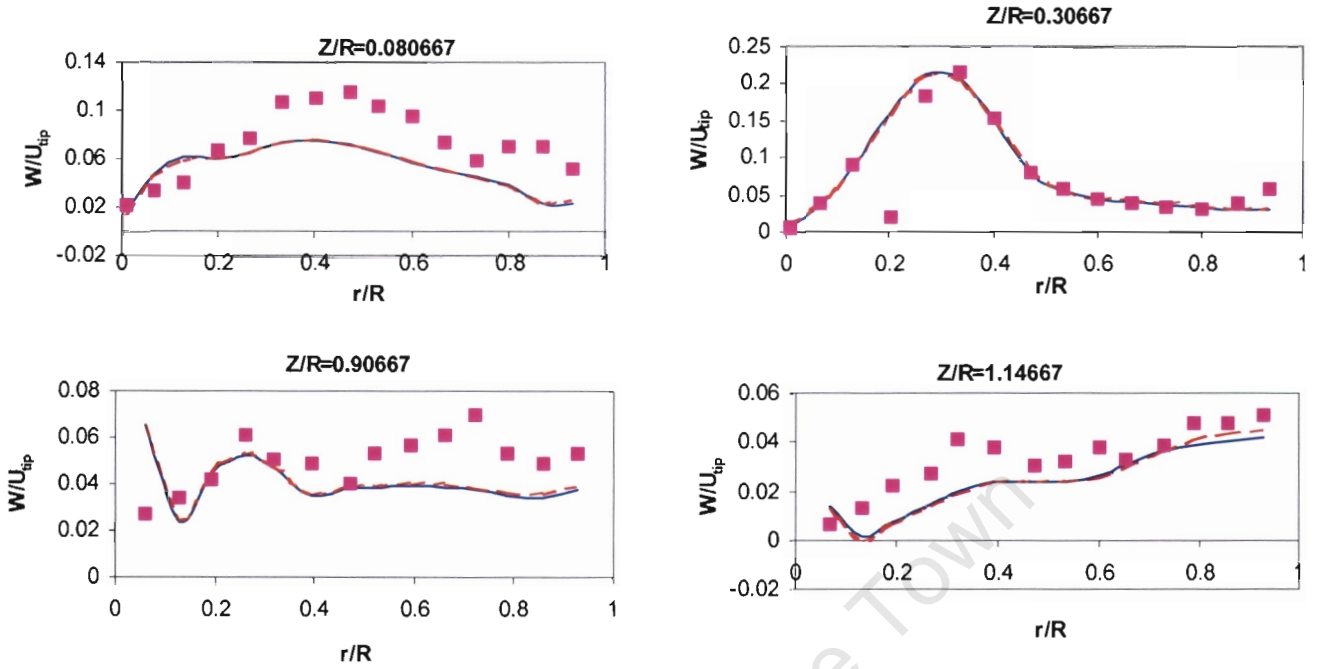


Figure G3: Tangential velocities of 45° pitched blade turbine with model parameters

$C_\mu=0.045$, $C_{\epsilon 1}=1.22$, $C_{\epsilon 2}=1.95$: ■ LDA, — Standard $k-\epsilon$ model, - - - Optimum model parameters

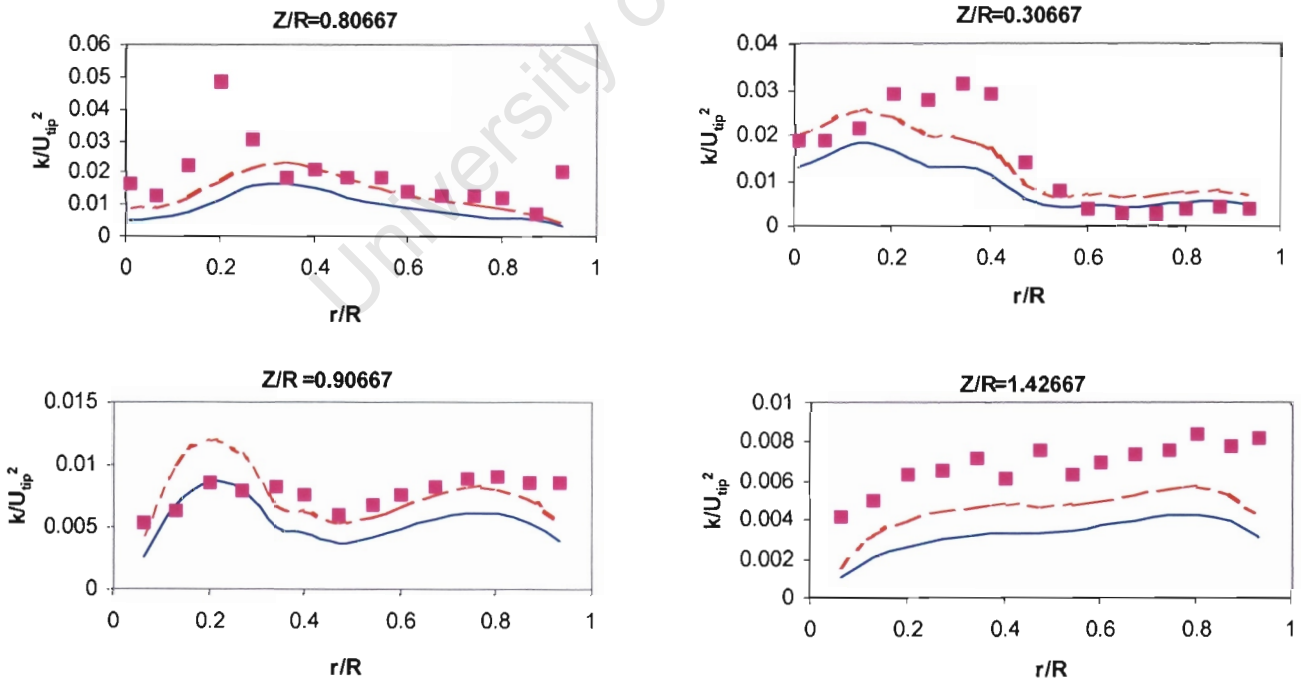


Figure G4: Turbulent kinetic energy of 45° pitched blade turbine with model parameters

$C_\mu=0.045$, $C_{\epsilon 1}=1.22$, $C_{\epsilon 2}=1.95$: ■ LDA, — Standard $k-\epsilon$ model, - - - Optimum model parameters

$C_\mu = 0.045$, $C_{\epsilon 1} = 1.4$, $C_{\epsilon 2} = 2.2$

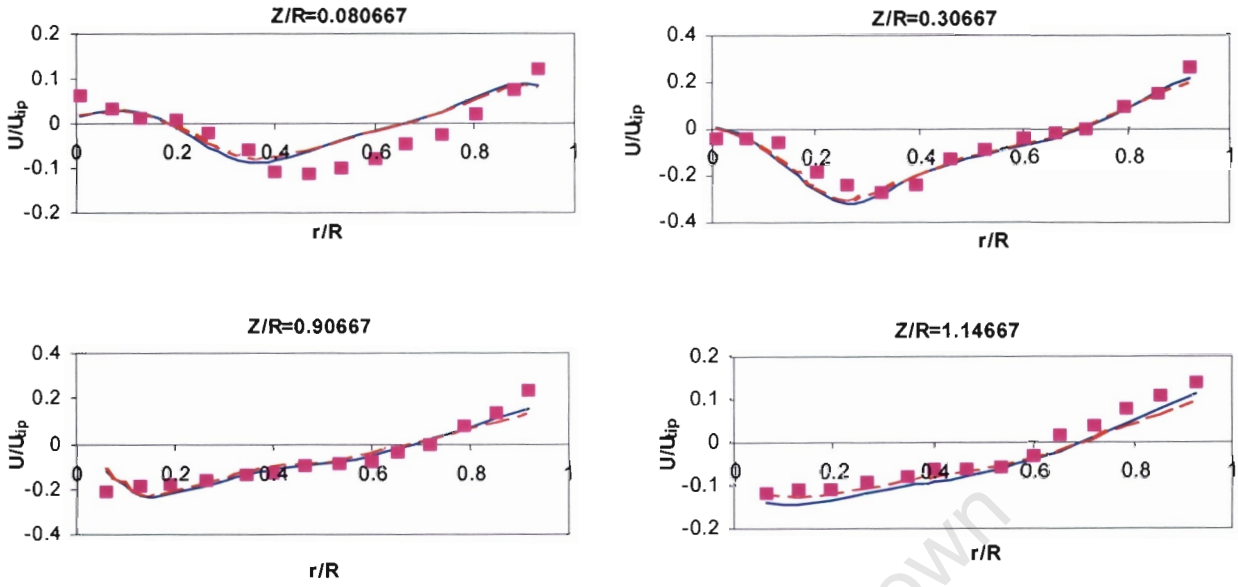


Figure G5: Axial velocities of 45° pitched blade turbine with model parameters $C_\mu = 0.045$, $C_{\epsilon 1} = 1.4$, $C_{\epsilon 2} = 2.2$: ■ LDA, — Standard $k-\epsilon$ model, - - - Optimum model parameters

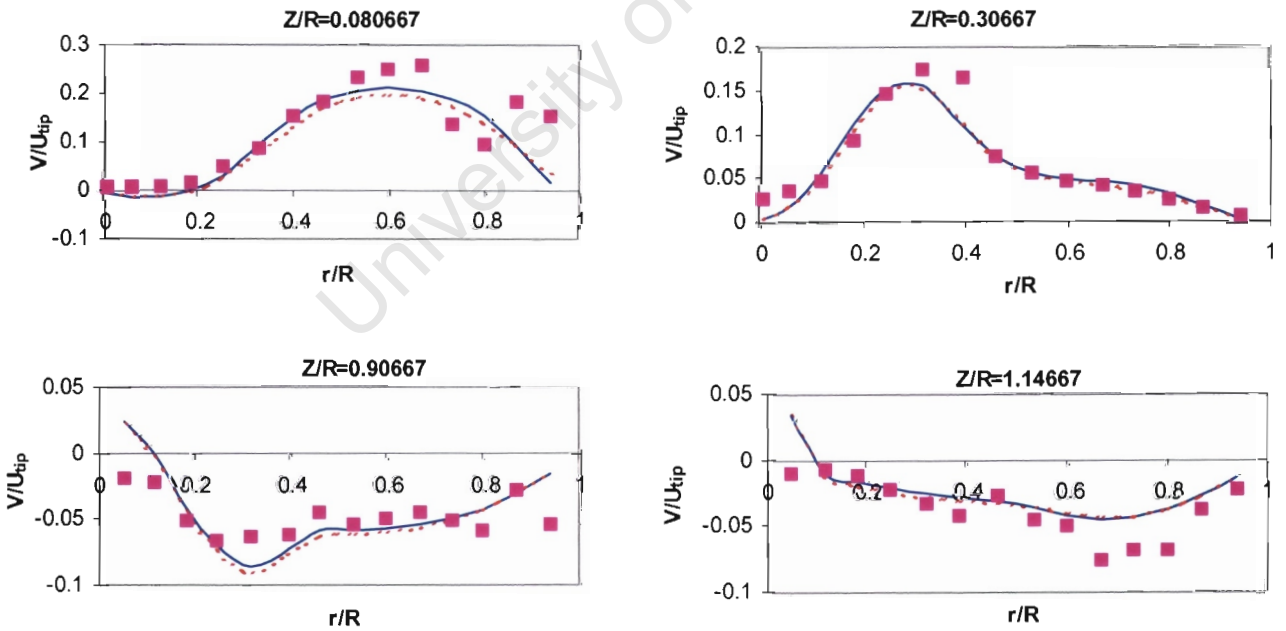


Figure G6: Radial velocities of 45° pitched blade turbine with model parameters $C_\mu = 0.045$, $C_{\epsilon 1} = 1.4$, $C_{\epsilon 2} = 2.2$: ■ LDA, — Standard $k-\epsilon$ model, - - - Optimum model parameters

$$C_\mu = 0.045, C_{\epsilon 1} = 1.4, C_{\epsilon 2} = 2.2$$

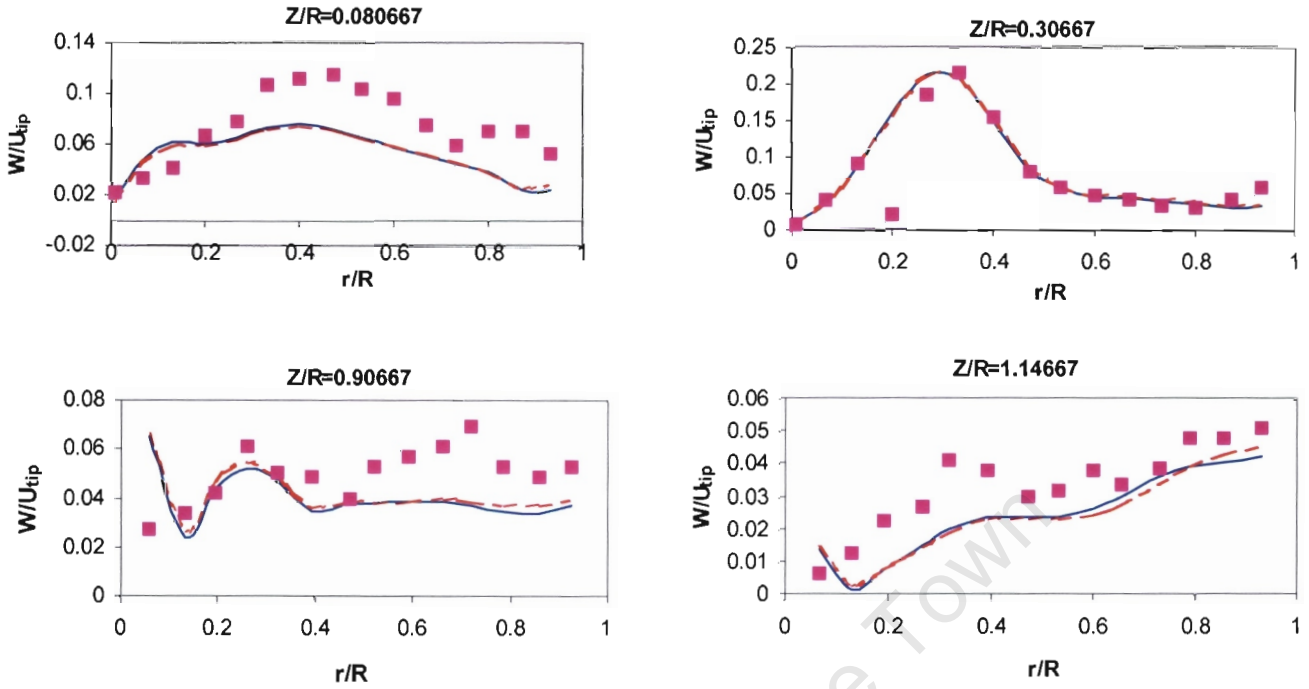


Figure G7: Tangential velocities of 45° pitched blade turbine with model parameters $C_\mu = 0.045$, $C_{\epsilon 1} = 1.4$, $C_{\epsilon 2} = 2.2$: ■ LDA, — Standard $k-\epsilon$ model, - - - Optimum model parameters

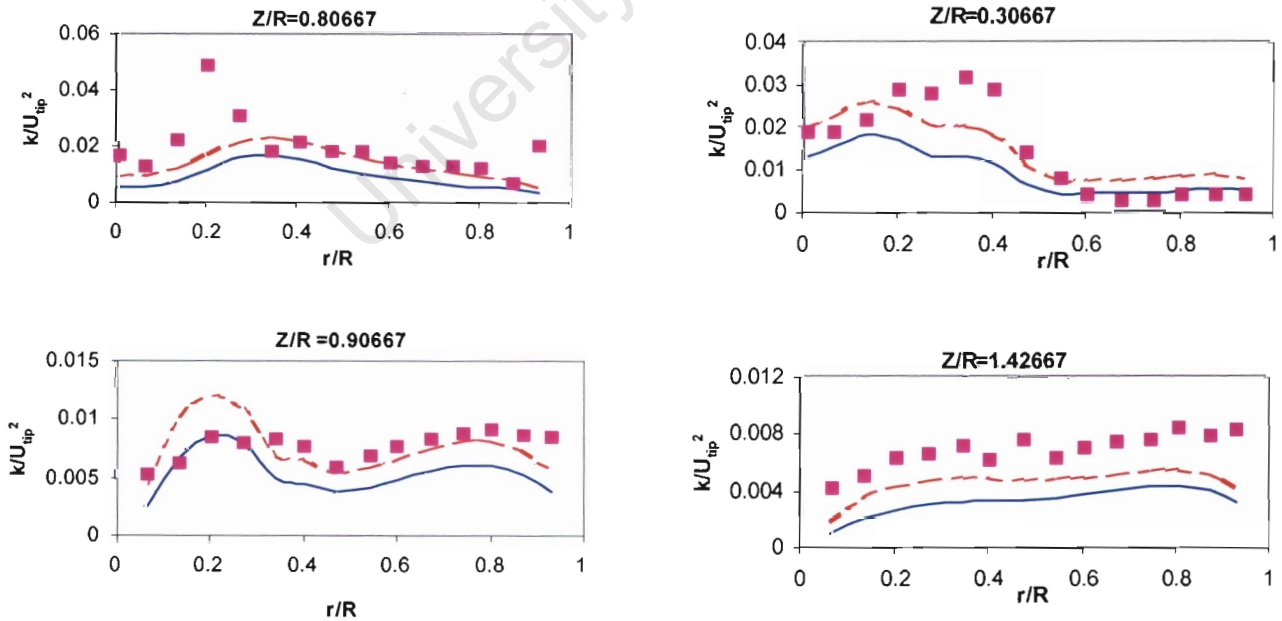


Figure G8: Turbulent kinetic energy of 45° pitched blade turbine with model parameters $C_\mu = 0.045$, $C_{\epsilon 1} = 1.4$, $C_{\epsilon 2} = 2.2$: ■ LDA, — Standard $k-\epsilon$ model, - - - Optimum model parameters

$$C_{\mu} = 0.09, C_{\varepsilon 1} = 1.22, C_{\varepsilon 2} = 1.75$$

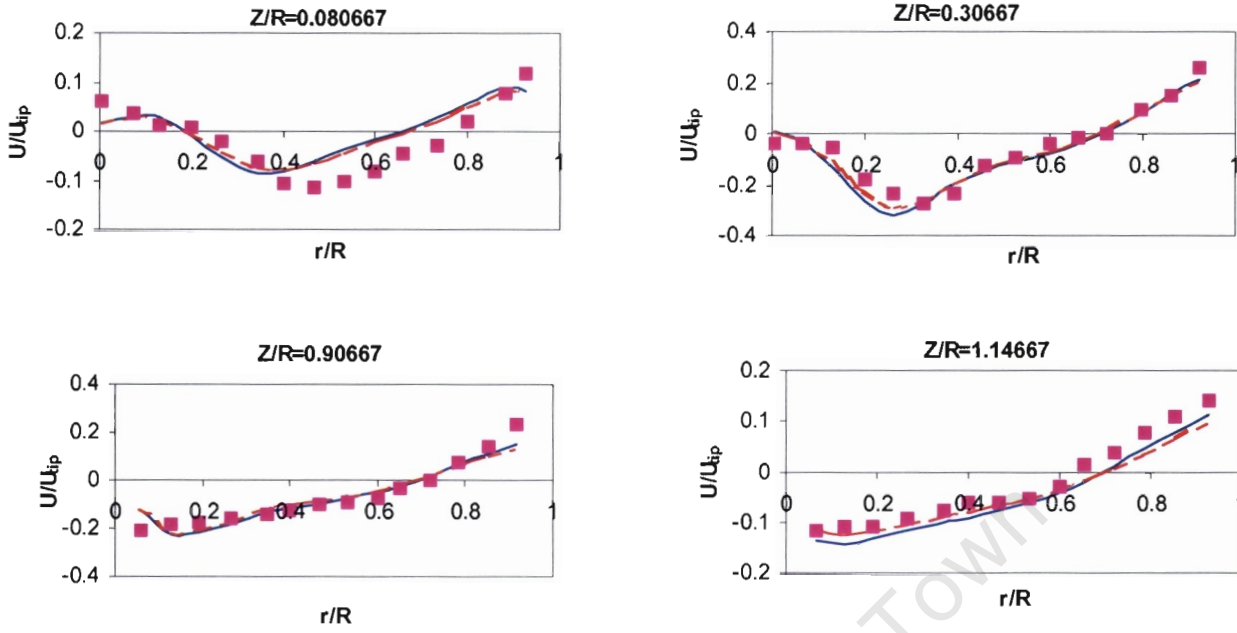


Figure G9: Axial velocities of 45° pitched blade turbine with model parameters $C_{\mu} = 0.09$, $C_{\varepsilon 1} = 1.22$, $C_{\varepsilon 2} = 1.75$: ■ LDA, — Standard $k-\varepsilon$ model, - - - Optimum model parameters

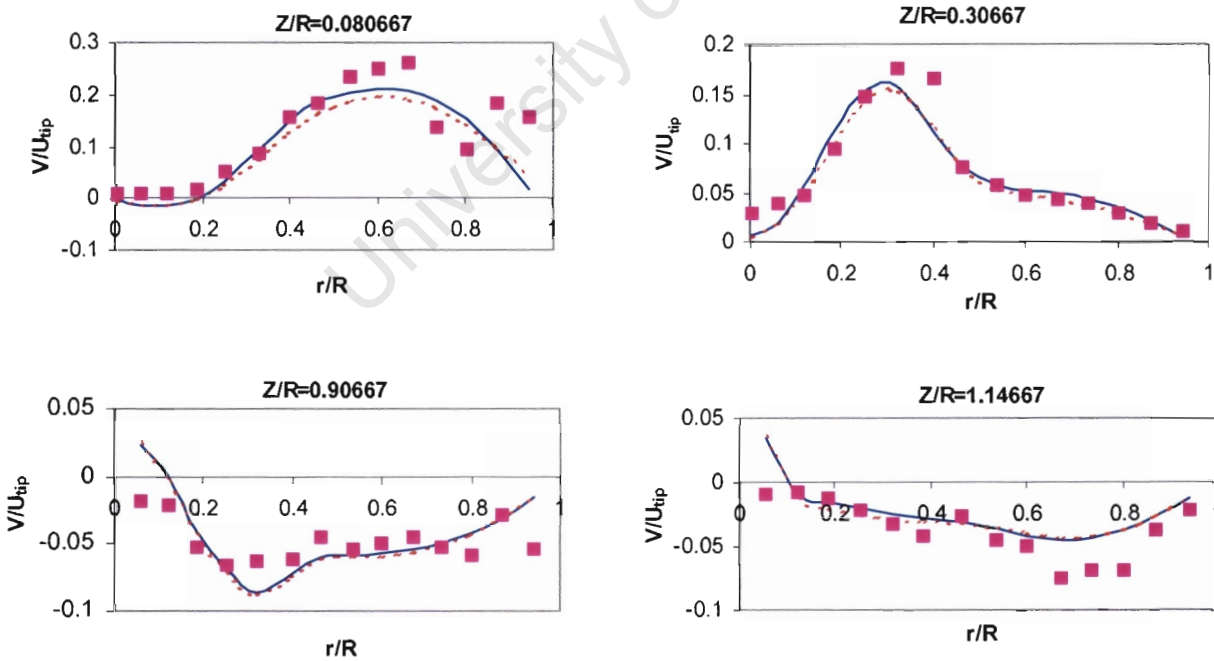


Figure G10: Radial velocities of 45° pitched blade turbine with model parameters $C_{\mu} = 0.09$, $C_{\varepsilon 1} = 1.22$, $C_{\varepsilon 2} = 1.75$: ■ LDA, — Standard $k-\varepsilon$ model, - - - Optimum model parameters

$$C_{\mu} = 0.09 \quad C_{\epsilon 1} = 1.22 \quad C_{\epsilon 2} = 1.75$$

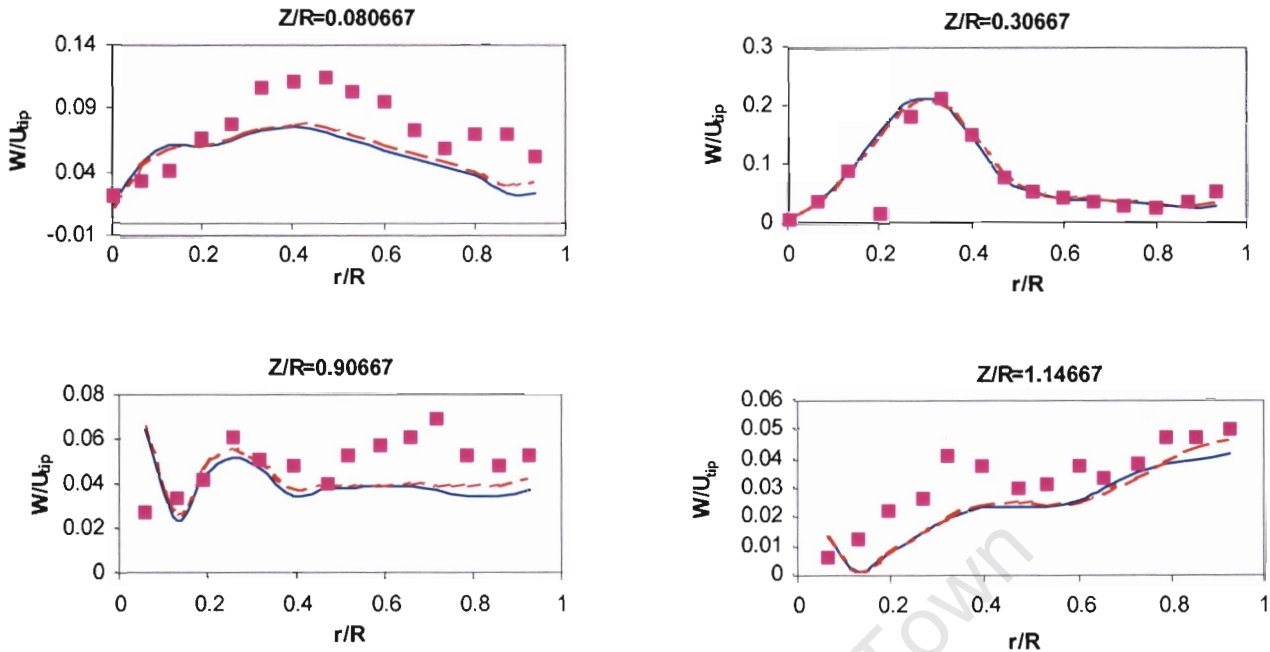


Figure G11: Tangential velocities of 45° pitched blade turbine with model parameters

$C_{\mu} = 0.09, C_{\epsilon 1} = 1.22 \quad C_{\epsilon 2} = 1.75$: ■ LDA, — Standard $k-\epsilon$ model, - - - Optimum model parameters

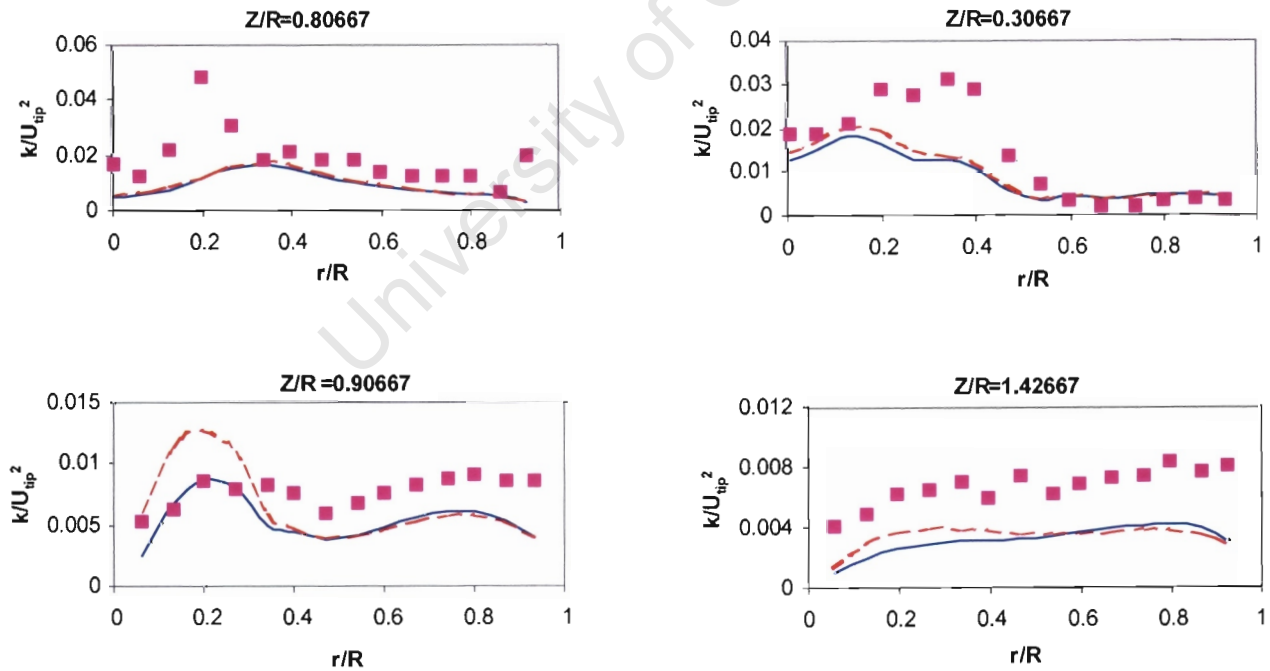


Figure G12: Turbulent kinetic energy of 45° pitched blade turbine with model parameters

$C_{\mu} = 0.09, C_{\epsilon 1} = 1.22 \quad C_{\epsilon 2} = 1.75$: ■ LDA, — Standard $k-\epsilon$ model, - - - Optimum model parameters

APPENDIX H

Performance of the optimum turbulence model parameters in Rushton turbine

$$C_{\mu} = 0.045 \quad C_{\epsilon 1} = 1.39, \quad C_{\epsilon 2} = 2.15$$

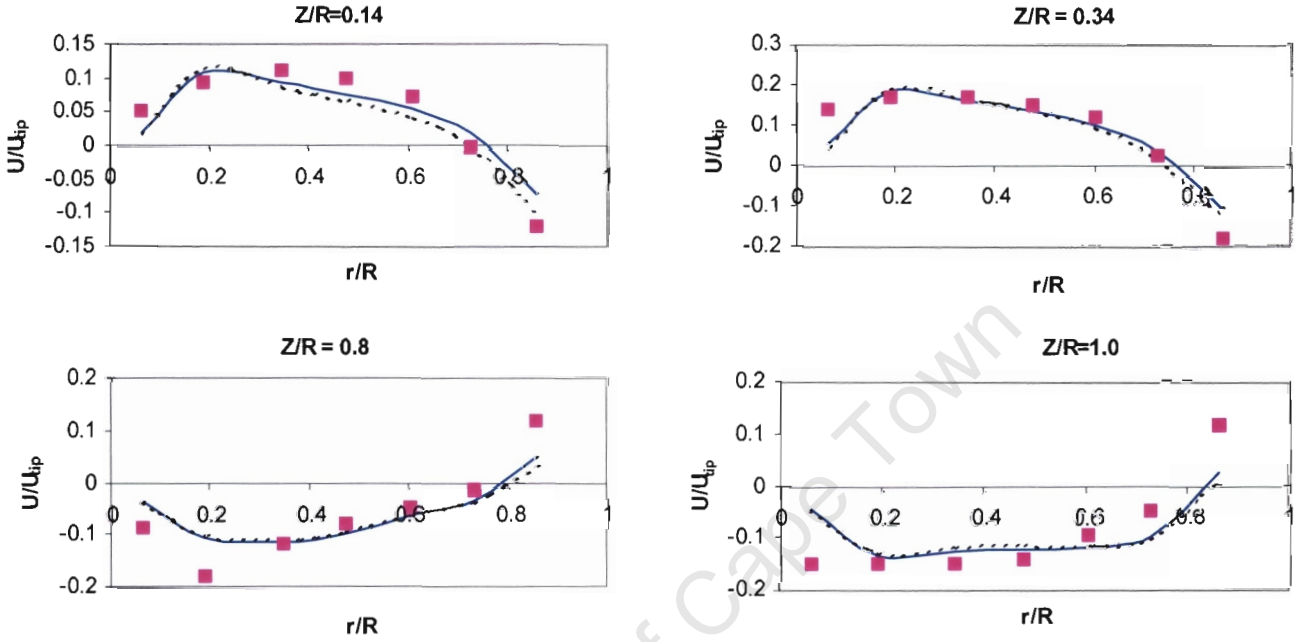


Figure H1: Axial velocities of Rushton turbine with model parameters $C_{\mu}=0.045$, $C_{\epsilon 1}=1.39$, $C_{\epsilon 2}=2.15$: ■ LDA, ---- Standard $k-\epsilon$ model, — Optimum model parameters

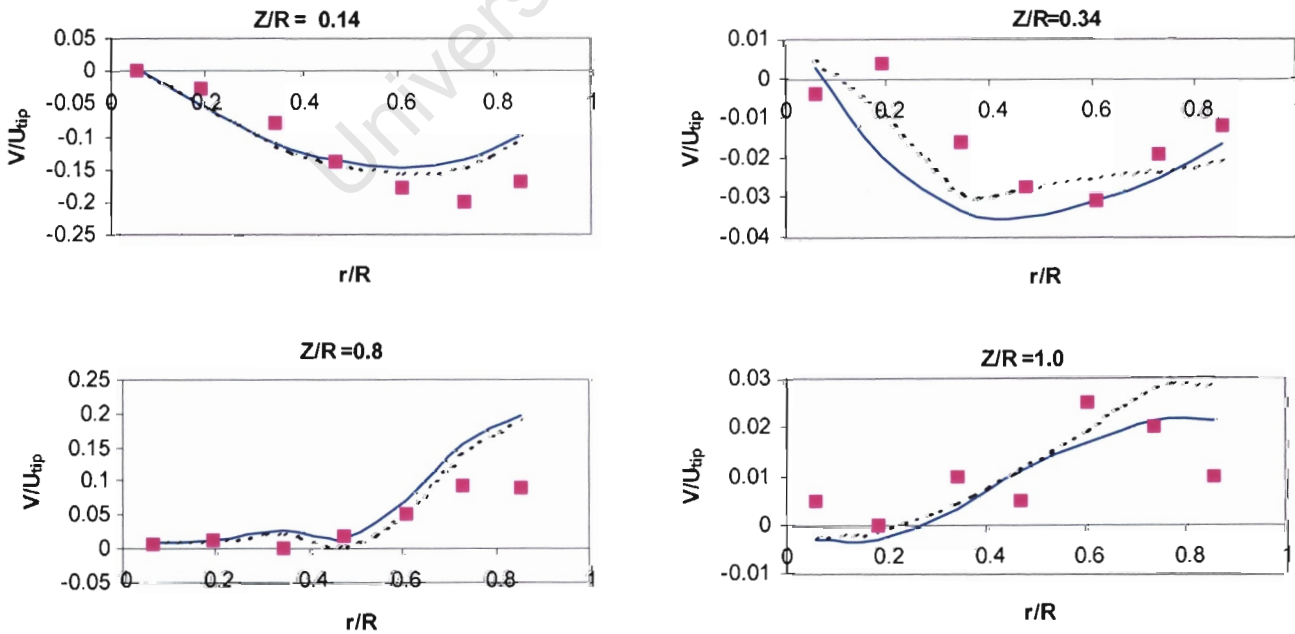


Figure H2: Radial velocities of Rushton turbine with model parameters $C_{\mu}=0.045$, $C_{\epsilon 1}=1.39$, $C_{\epsilon 2}=2.15$: ■ LDA, ---- Standard $k-\epsilon$ model, — Optimum model parameters

$$C_{\mu} = 0.045, C_{\epsilon 1} = 1.39, C_{\epsilon 2} = 2.15$$

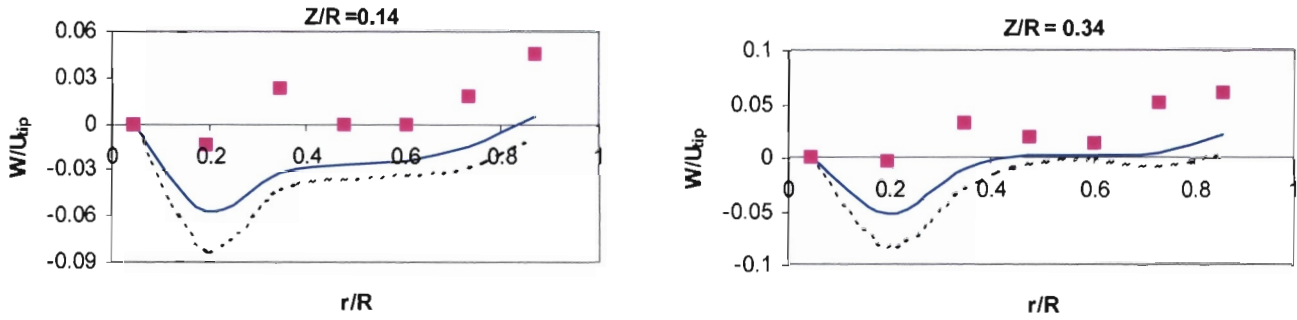


Figure H3: Tangential velocities of Rushton turbine with model parameters $C_{\mu}=0.045$, $C_{\epsilon 1}=1.39$, $C_{\epsilon 2}=2.15$: ■ LDA, ---- Standard $k-\epsilon$ model, — Optimum model parameters

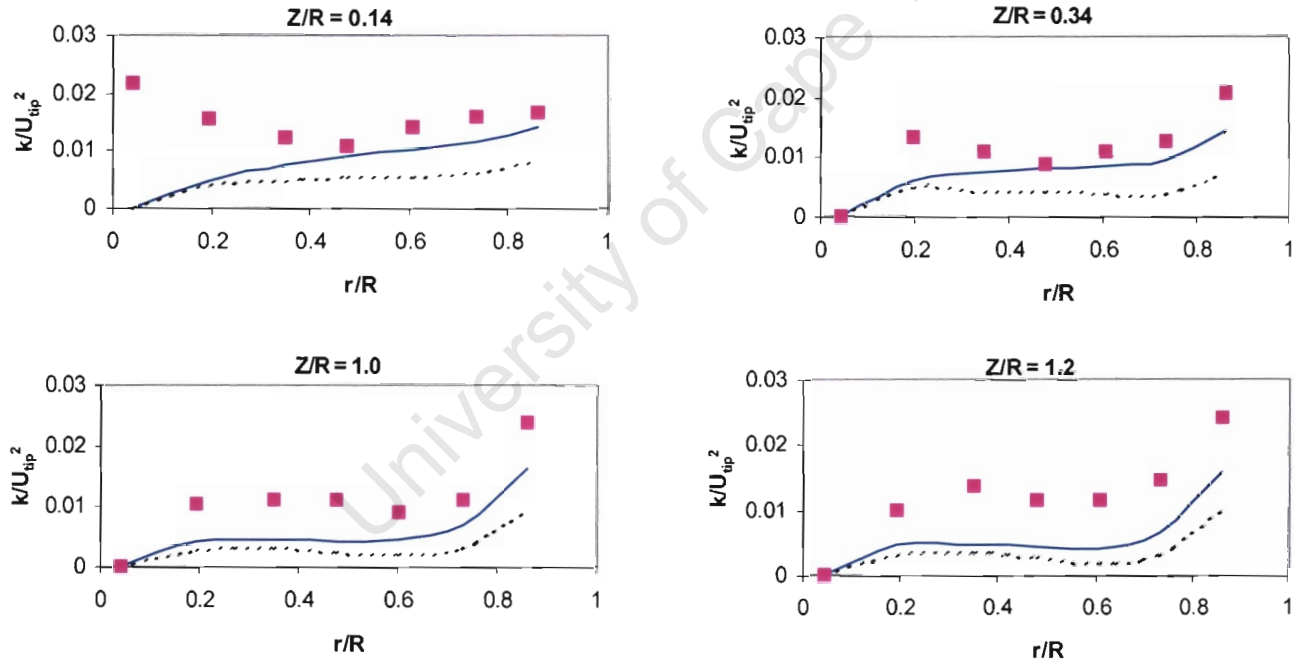


Figure H4: Turbulent kinetic energy of Rushton turbine with model parameters $C_{\mu} = 0.045$, $C_{\epsilon 1}=1.39$, $C_{\epsilon 2}=2.15$: ■ LDA, ---- Standard $k-\epsilon$ model, — Optimum model parameters

$$C_\mu = 0.07, C_{\varepsilon 1} = 1.4, C_{\varepsilon 2} = 2$$

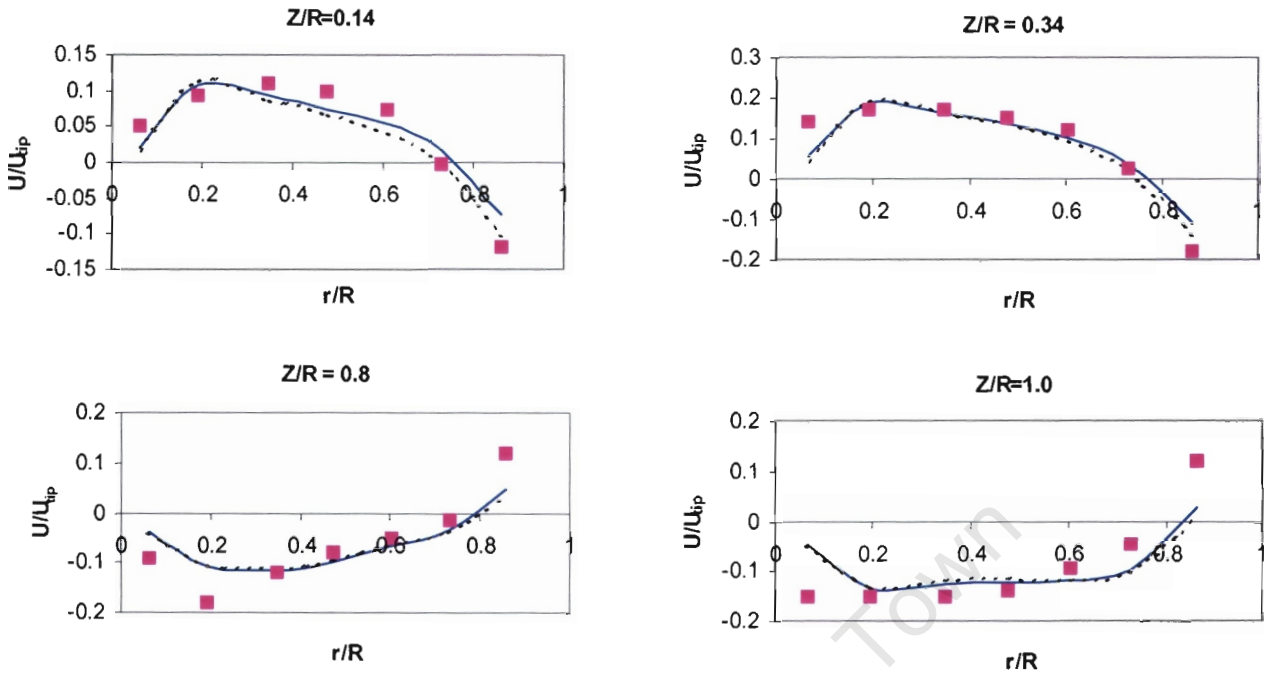


Figure H5: Axial velocities of Rushton turbine with model parameters $C_\mu = 0.07$, $C_{\varepsilon 1} = 1.4$, $C_{\varepsilon 2} = 2$: ■ LDA, ---- Standard $k-\varepsilon$ model, — Optimum model parameters

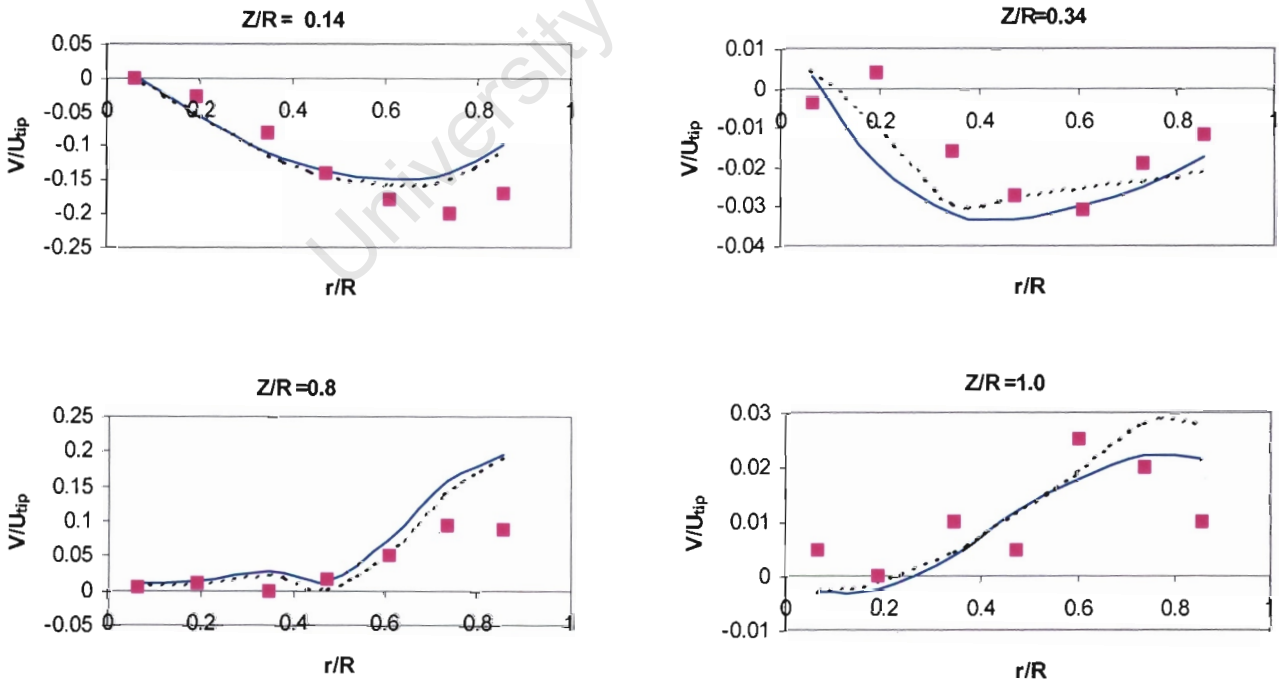


Figure H6: Radial velocities of Rushton turbine with model parameters $C_\mu = 0.07$, $C_{\varepsilon 1} = 1.4$, $C_{\varepsilon 2} = 2$: ■ LDA, ---- Standard $k-\varepsilon$ model, — Optimum model parameters

$$C_{\mu} = 0.07, C_{\varepsilon 1} = 1.4, C_{\varepsilon 2} = 2$$

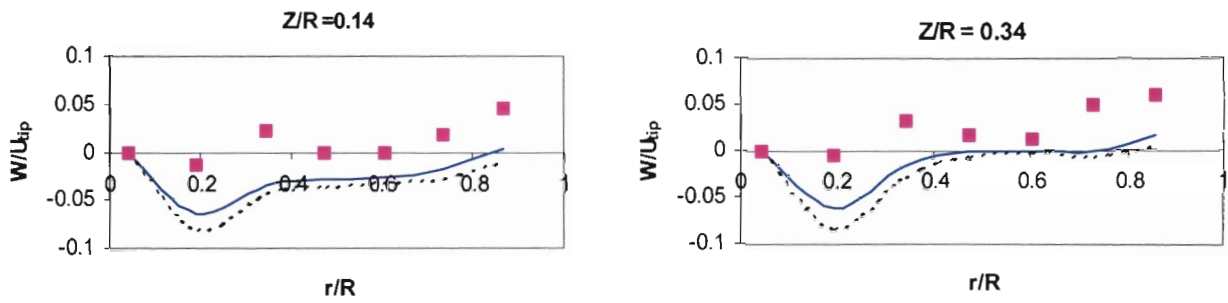


Figure H7: Tangential velocities of Rushton turbine with model parameters $C_{\mu} = 0.07$, $C_{\varepsilon 1} = 1.4$, $C_{\varepsilon 2} = 2$: $\blacksquare$ LDA, ---- Standard $k-\varepsilon$ model, — Optimum model parameters

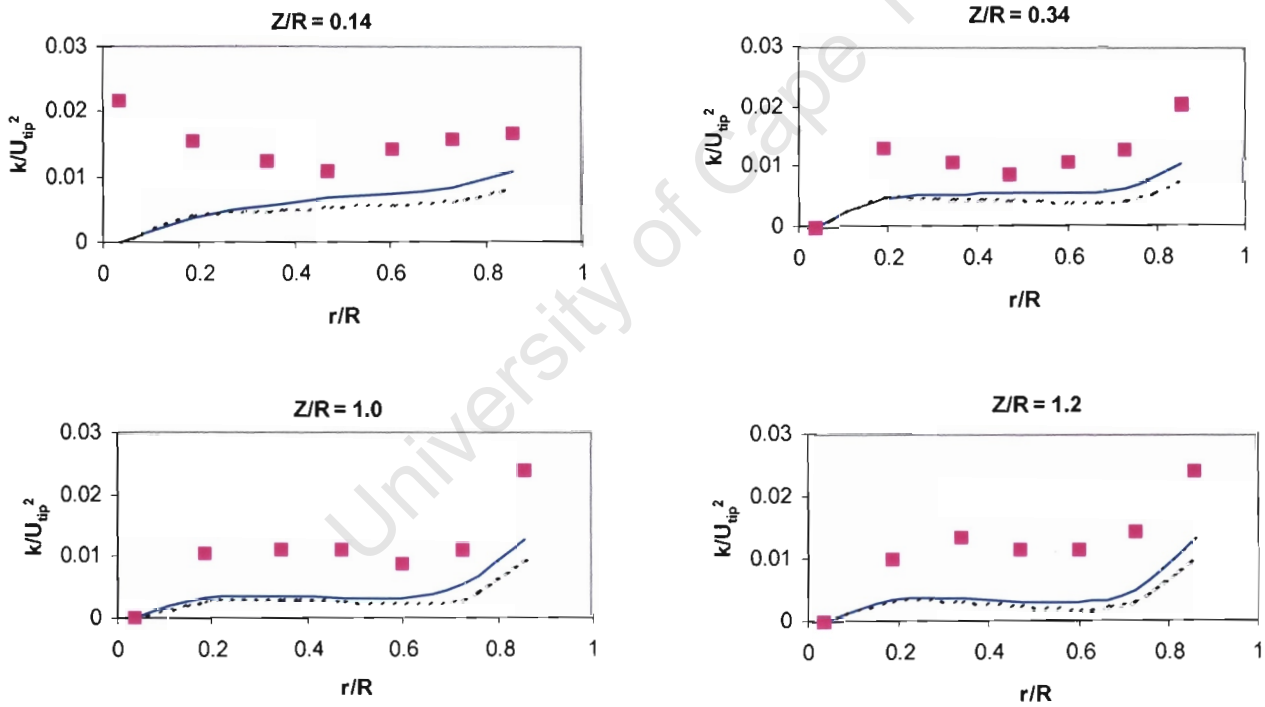


Figure H8: Turbulent kinetic energy of Rushton turbine with model parameters $C_{\mu} = 0.07$, $C_{\varepsilon 1} = 1.4$, $C_{\varepsilon 2} = 2$: $\blacksquare$ LDA, ---- Standard $k-\varepsilon$ model, — Optimum model parameters

APPENDIX I

Performance of the optimum turbulence model parameters in 30° Pitched blade turbine

$C_\mu=0.045$, $C_{\varepsilon 1}=1.25$, $C_{\varepsilon 2}=2$:

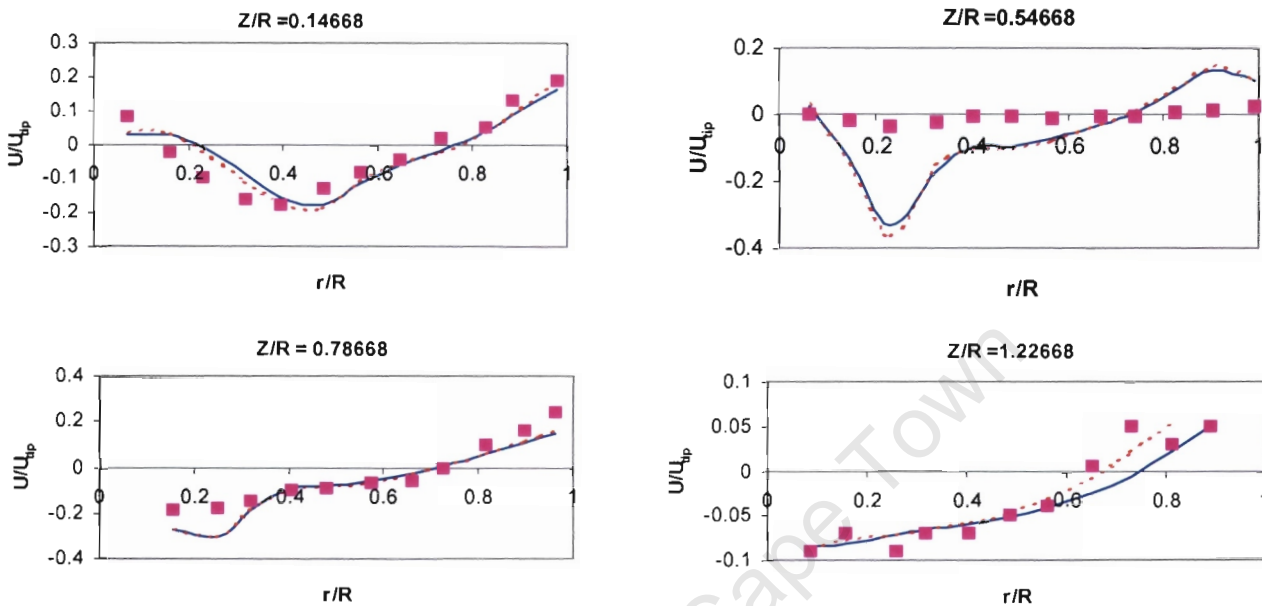


Figure I1: Axial velocities of 30° pitched blade turbine with model parameters $C_\mu=0.045$, $C_{\varepsilon 1}=1.25$, $C_{\varepsilon 2}=2$: ■ LDA, --- Standard $k-\varepsilon$ model, — Optimum model parameters

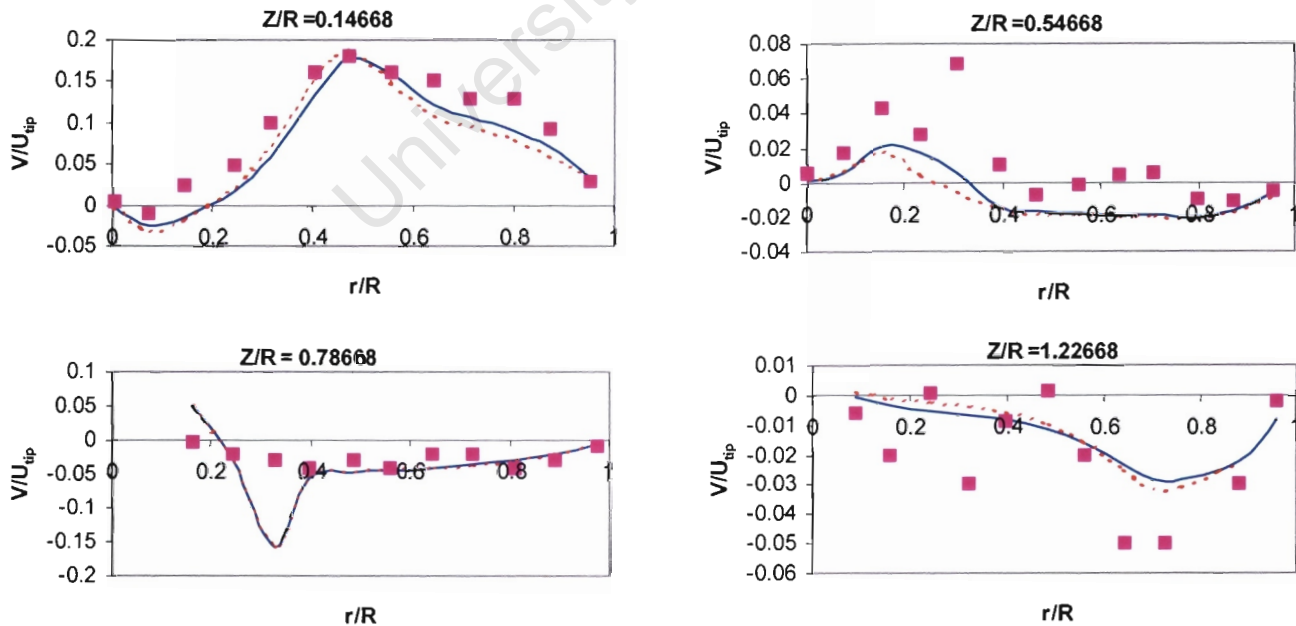


Figure I2: Radial velocities of 30° pitched blade turbine with model parameters $C_\mu=0.045$, $C_{\varepsilon 1}=1.25$, $C_{\varepsilon 2}=2$: ■ LDA, --- Standard $k-\varepsilon$ model, — Optimum model parameters

$$C_\mu = 0.045, C_{\epsilon 1} = 1.25, C_{\epsilon 2} = 2$$

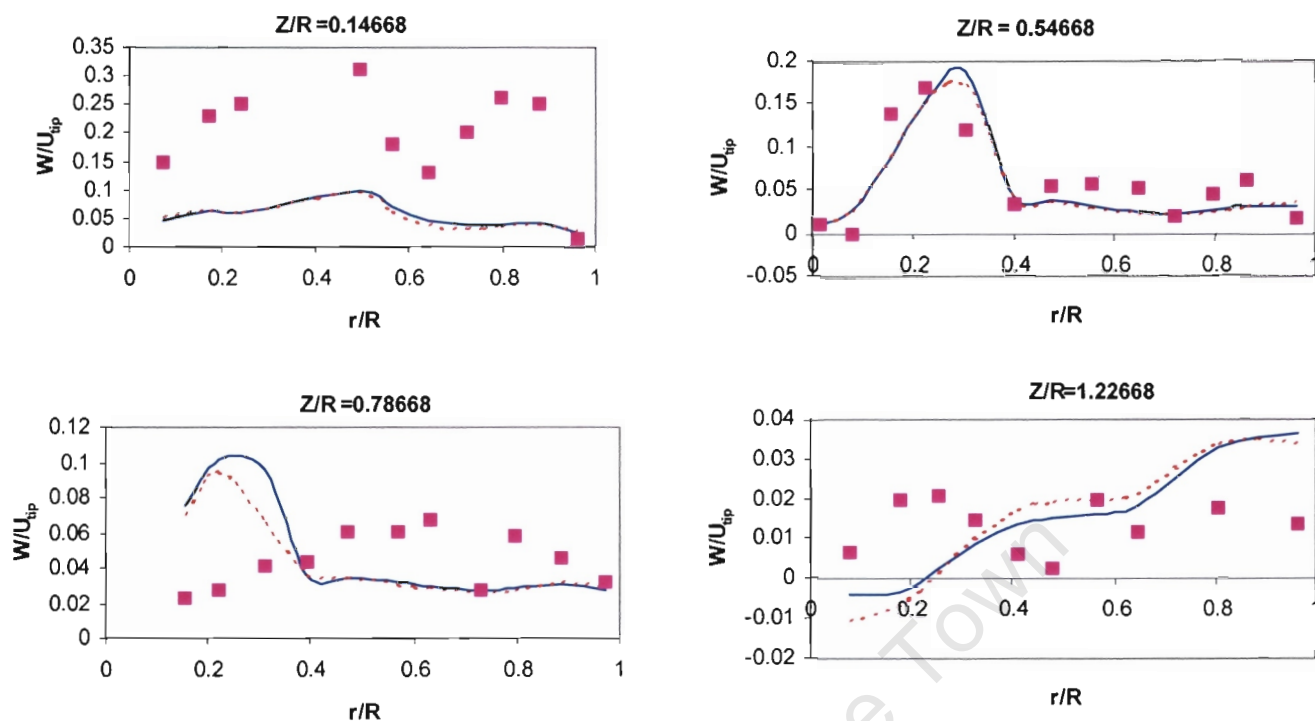


Figure I3: Tangential velocities of 30° pitched blade turbine with model parameters

$$C_\mu = 0.045, C_{\epsilon 1} = 1.25, C_{\epsilon 2} = 2: \quad \blacksquare \text{ LDA, } \text{---} \text{ Standard } k-\epsilon \text{ model, } \text{—} \text{ Optimum model parameters}$$

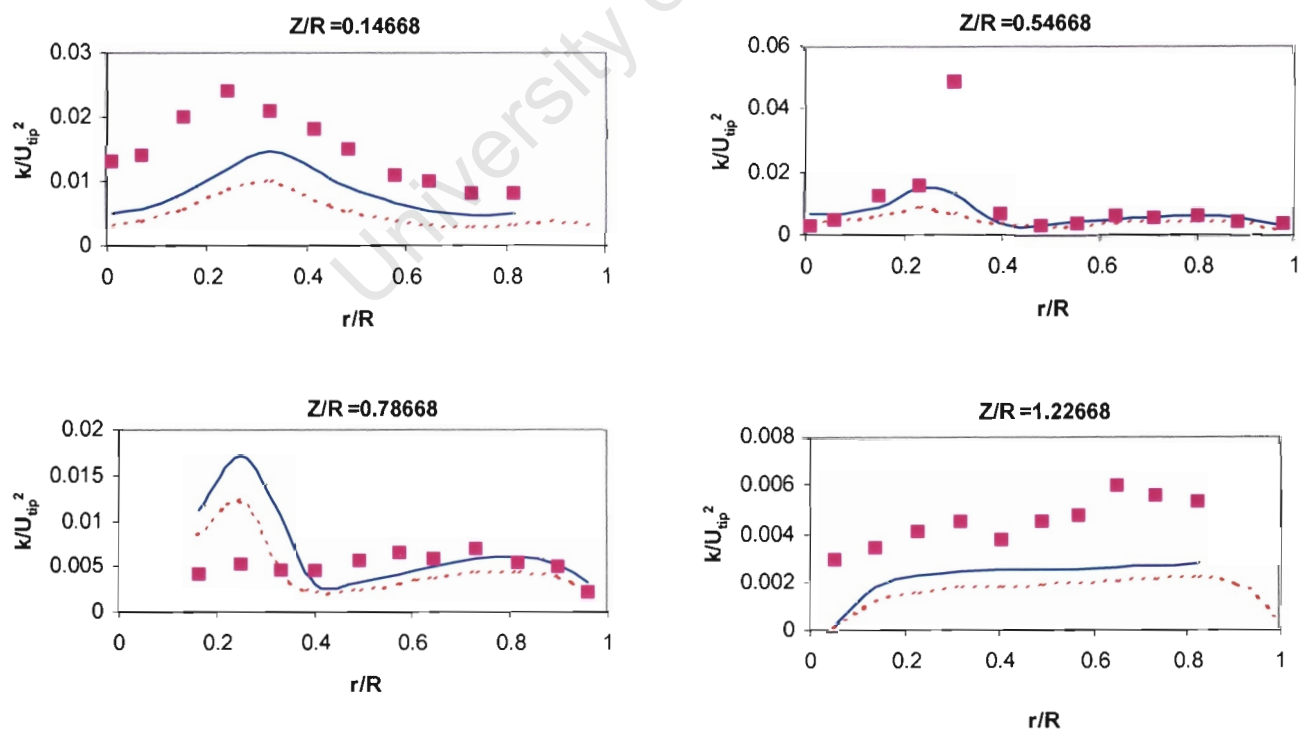


Figure I4: Turbulent kinetic energy of 30° pitched blade turbine with model parameters

$$C_\mu = 0.045, C_{\epsilon 1} = 1.25, C_{\epsilon 2} = 2: \quad \blacksquare \text{ LDA, } \text{---} \text{ Standard } k-\epsilon \text{ model, } \text{—} \text{ Optimum model parameters}$$

$$C_{\mu} = 0.0675, C_{\varepsilon 1} = 1.31, C_{\varepsilon 2} = 1.95$$

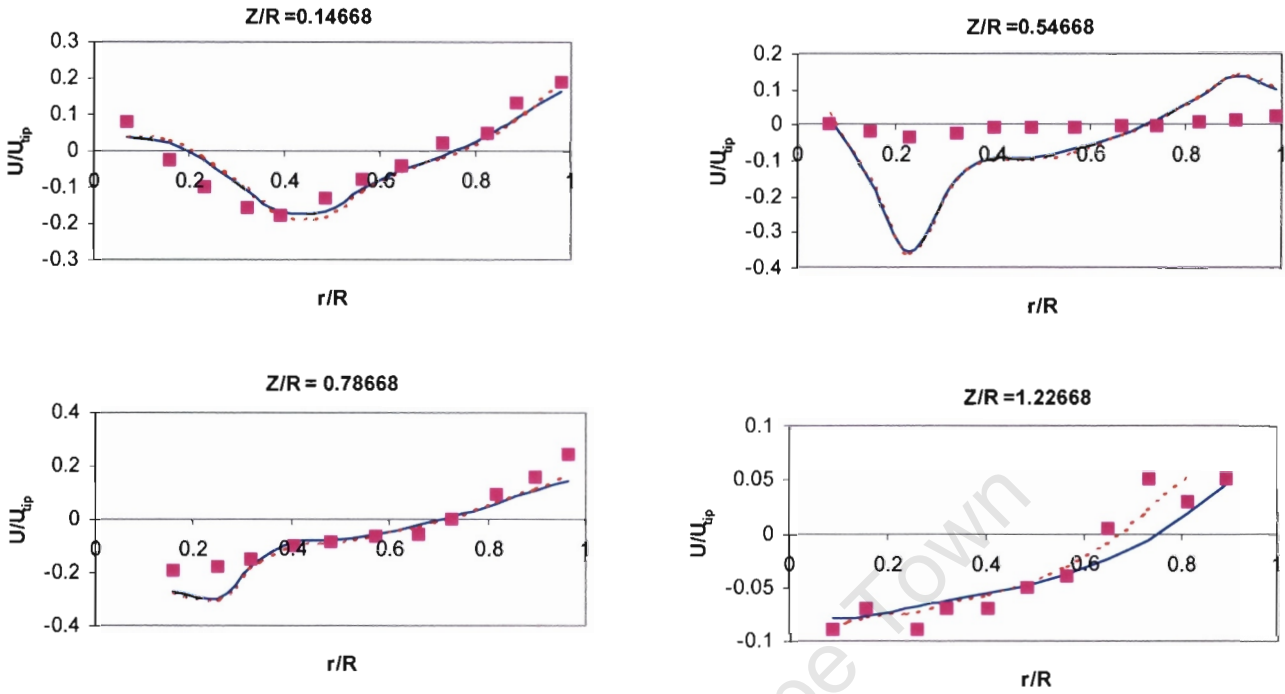


Figure I5: Axial velocities of 30° pitched blade turbine with model parameters $C_{\mu} = 0.0675$, $C_{\varepsilon 1} = 1.31$, $C_{\varepsilon 2} = 1.95$: ■ LDA, --- Standard $k-\varepsilon$ model, — Optimum model parameters

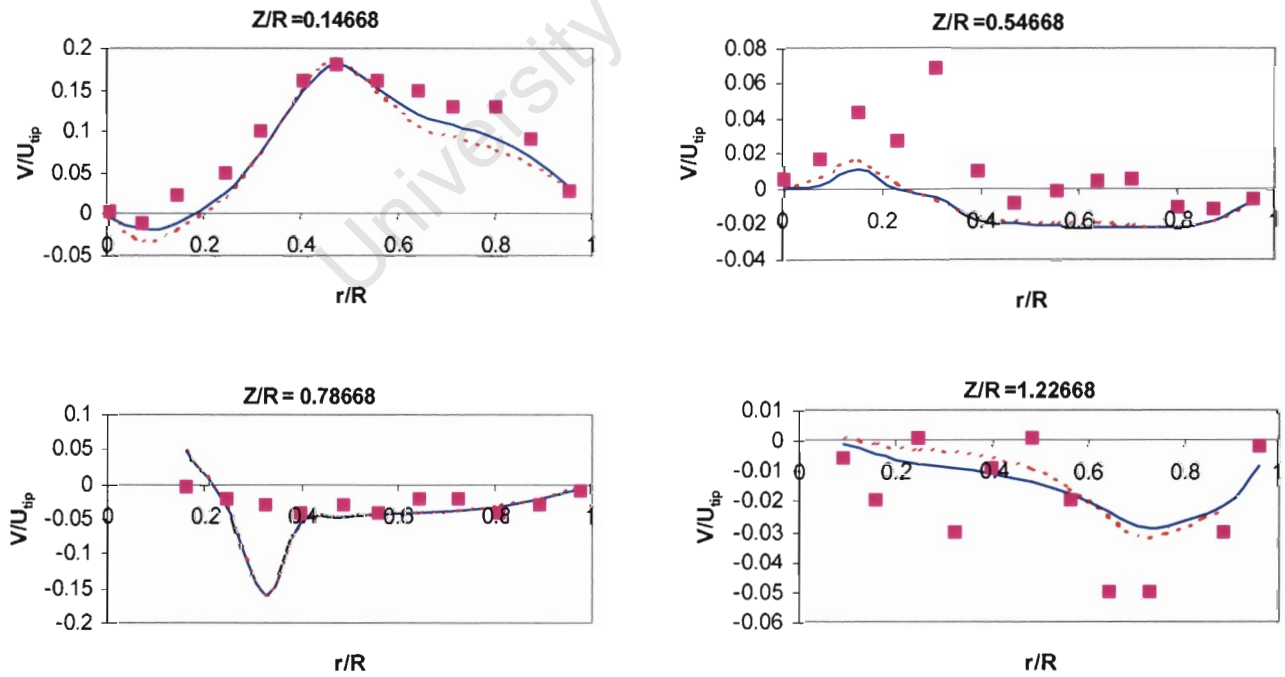


Figure I6: Radial velocities of 30° pitched blade turbine with model parameters $C_{\mu} = 0.0675$, $C_{\varepsilon 1} = 1.31$, $C_{\varepsilon 2} = 1.95$: ■ LDA, --- Standard $k-\varepsilon$ model, — Optimum model parameters

$C_\mu = 0.0675, C_{\epsilon 1} = 1.31, C_{\epsilon 2} = 1.95$

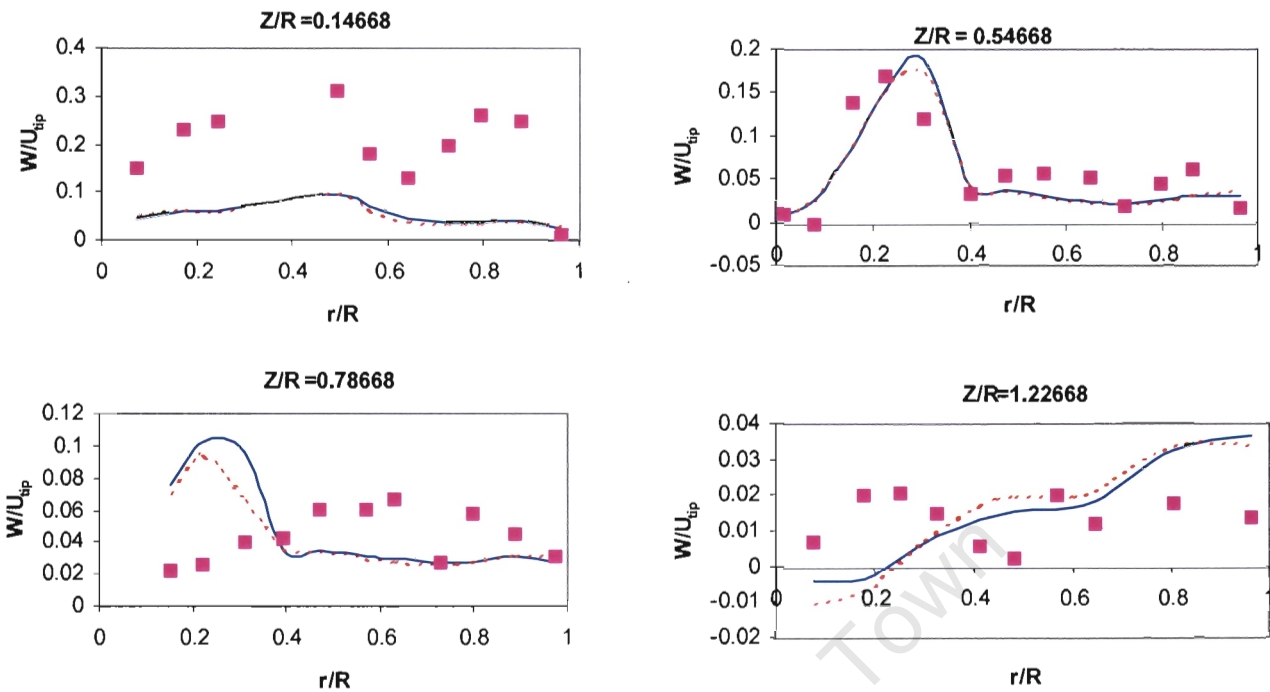


Figure I7: Tangential velocities of 30° pitched blade turbine with model parameters

$C_\mu = 0.0675, C_{\epsilon 1} = 1.31, C_{\epsilon 2} = 1.95$: ■ LDA, - - - Standard $k-\epsilon$ model, — Optimum model

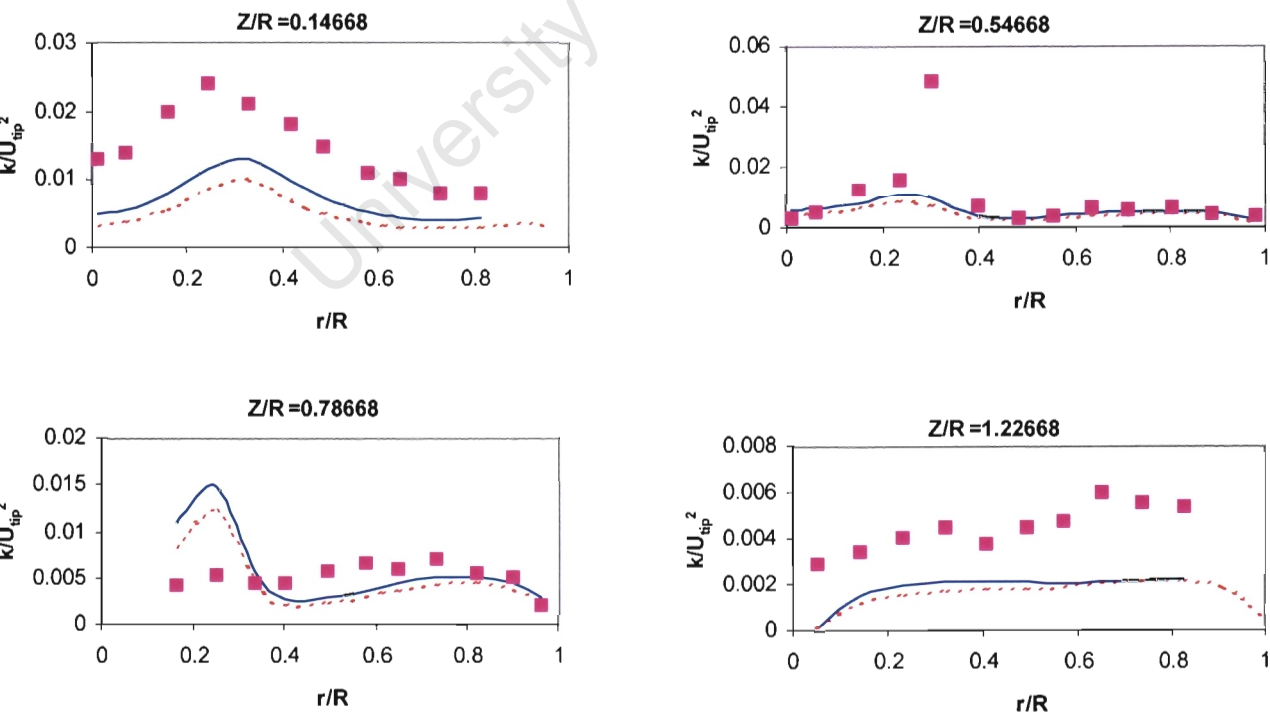


Figure I8: Turbulent kinetic energy of 30° pitched blade turbine with model parameters

$C_\mu = 0.0675, C_{\epsilon 1} = 1.31, C_{\epsilon 2} = 1.9$ ■ LDA, - - - Standard $k-\epsilon$ model, — Optimum model parameters

APPENDIX J

Performance of the optimum turbulence model parameters in 60° Pitched blade turbine

$C_\mu=0.065, C_{\epsilon1}=1.2, C_{\epsilon2}=1.8$

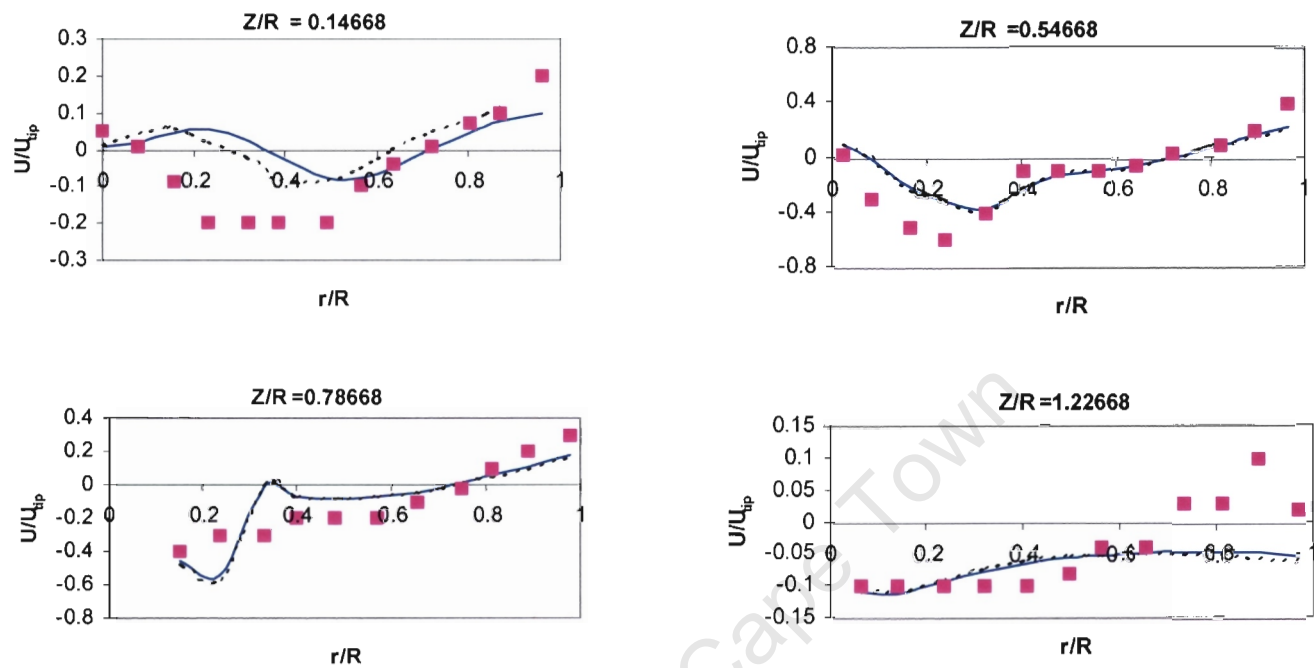


Figure J1: Axial velocities of 60° pitched blade turbine with model parameters $C_\mu=0.065, C_{\epsilon1}=1.2, C_{\epsilon2}=1.8$: ■ LDA, ---- Standard $k-\epsilon$ model . Optimum model parameters

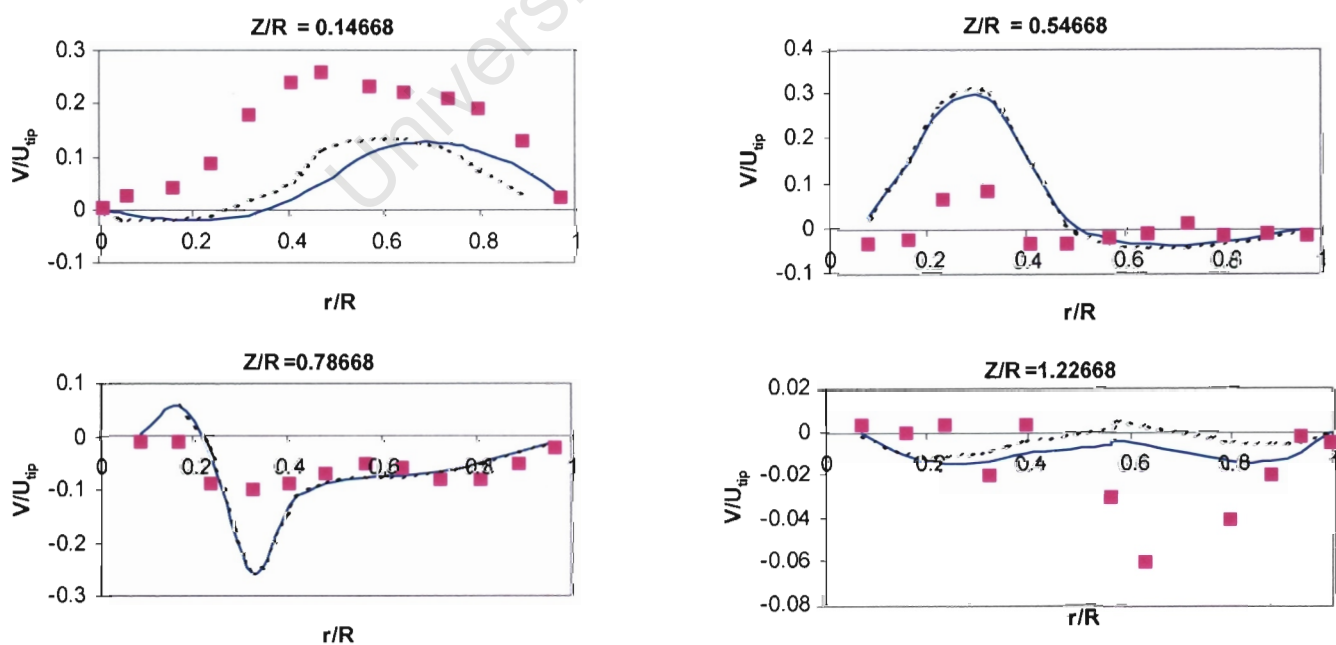


Figure J2: Radial velocities of 60° pitched blade turbine with model parameters $C_\mu=0.065, C_{\epsilon1}=1.2, C_{\epsilon2}=1.8$: ■ LDA, ---- Standard $k-\epsilon$ model . — Optimum model parameters

$C_{\mu}=0.065, C_{\epsilon 1}=1.2, C_{\epsilon 2}=1.8$

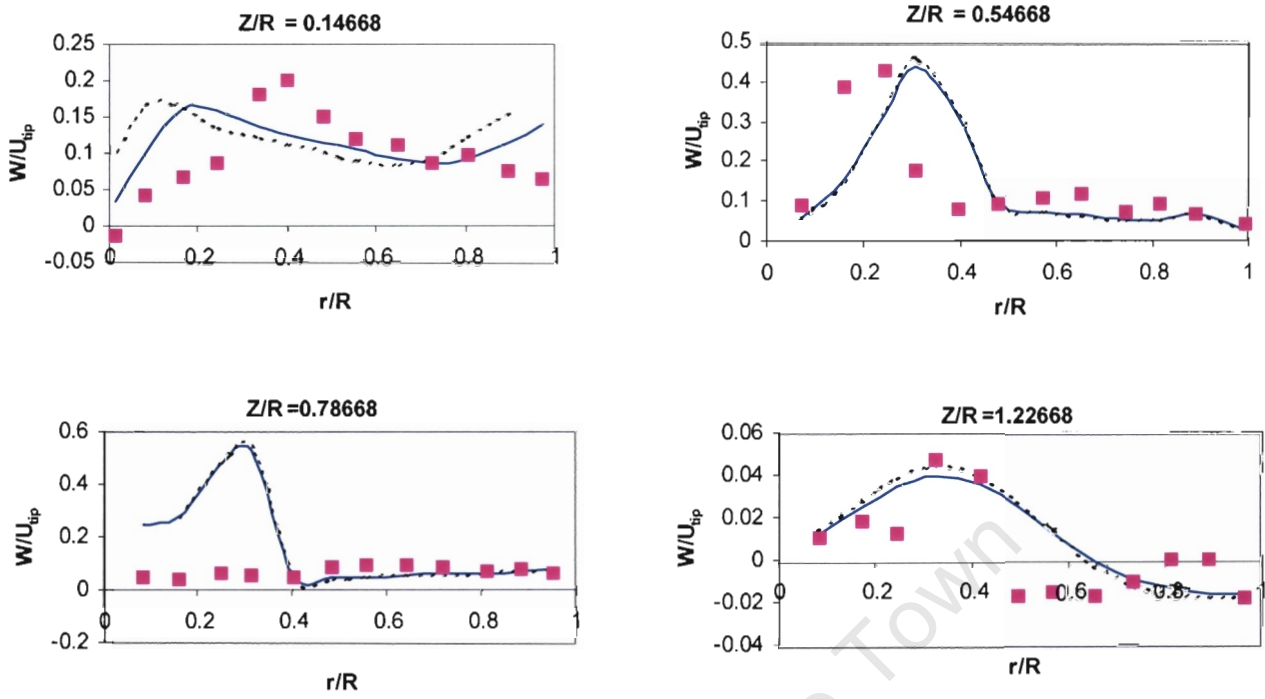


Figure J2: Tangential velocities of 60° pitched blade turbine with model parameters

$C_{\mu}=0.065, C_{\epsilon 1}=1.2, C_{\epsilon 2}=1.8$: ■ LDA, ---- Standard $k-\epsilon$ model. — Optimum model parameters

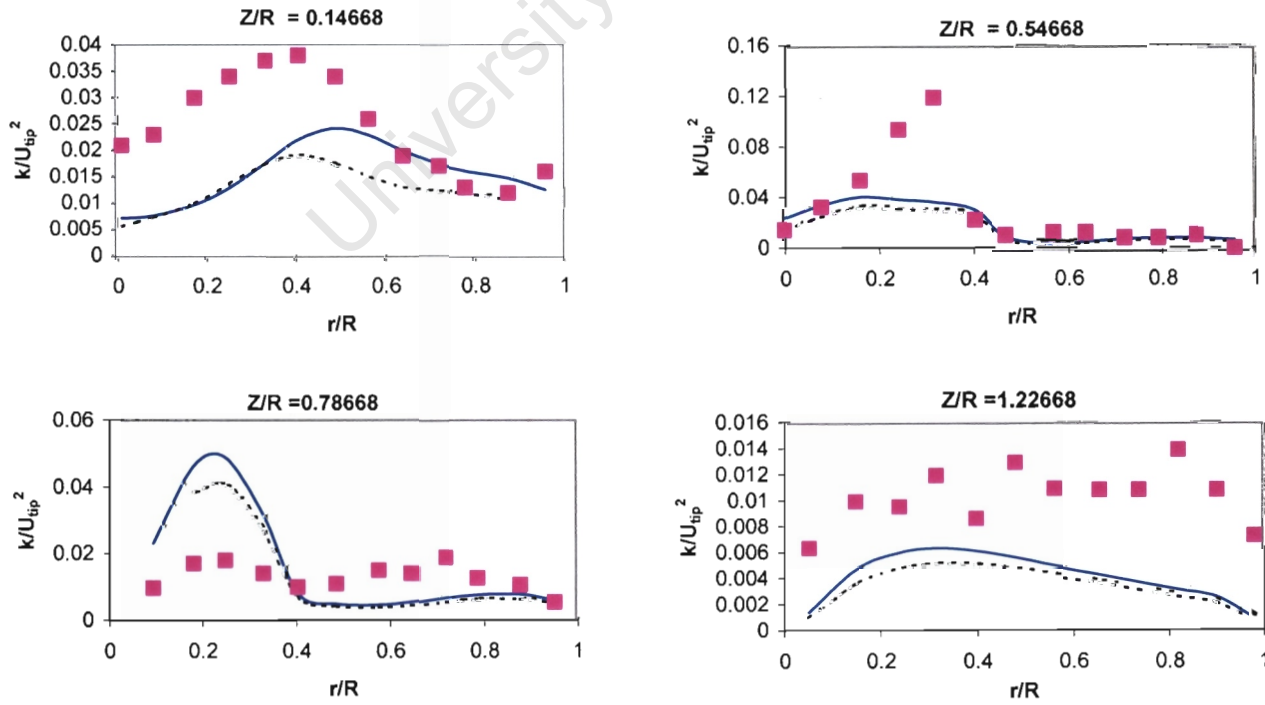


Figure J2: Turbulent kinetic energy of 60° pitched blade turbine with model parameters

$C_{\mu}=0.065, C_{\epsilon 1}=1.2, C_{\epsilon 2}=1.8$: ■ LDA, ---- Standard $k-\epsilon$ model. — Optimum model parameters

$C_\mu = 0.045, C_{\epsilon 1} = 1.25, C_{\epsilon 2} = 2$

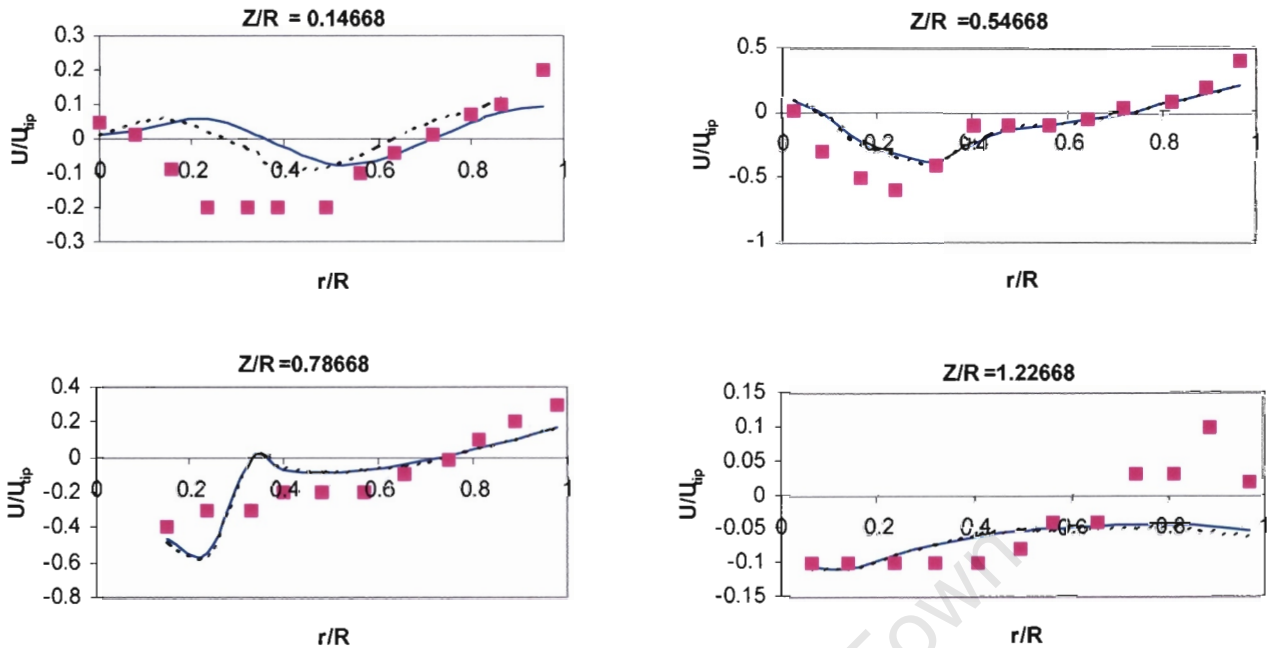


Figure J5: Axial velocities of 60° pitched blade turbine with model parameters $C_\mu=0.045$, $C_{\epsilon 1}=1.25$, $C_{\epsilon 2}=2$: ■ LDA, ---- Standard $k-\epsilon$ model. — Optimum model parameters

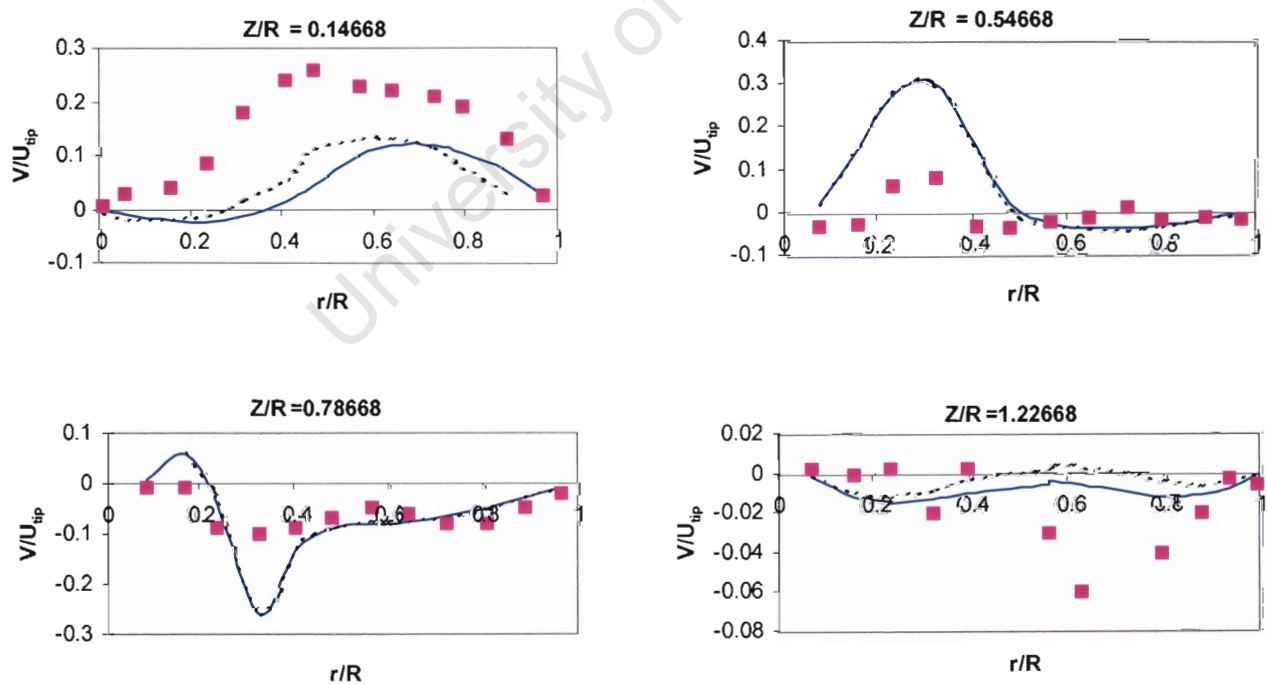


Figure J6: Radial velocities of 60° pitched blade turbine with model parameters $C_\mu=0.045$, $C_{\epsilon 1}=1.25$, $C_{\epsilon 2}=2$: ■ LDA, ---- Standard $k-\epsilon$ model. — Optimum model parameters

$C_{\mu} = 0.045, C_{\epsilon 1} = 1.25, C_{\epsilon 2} = 2$

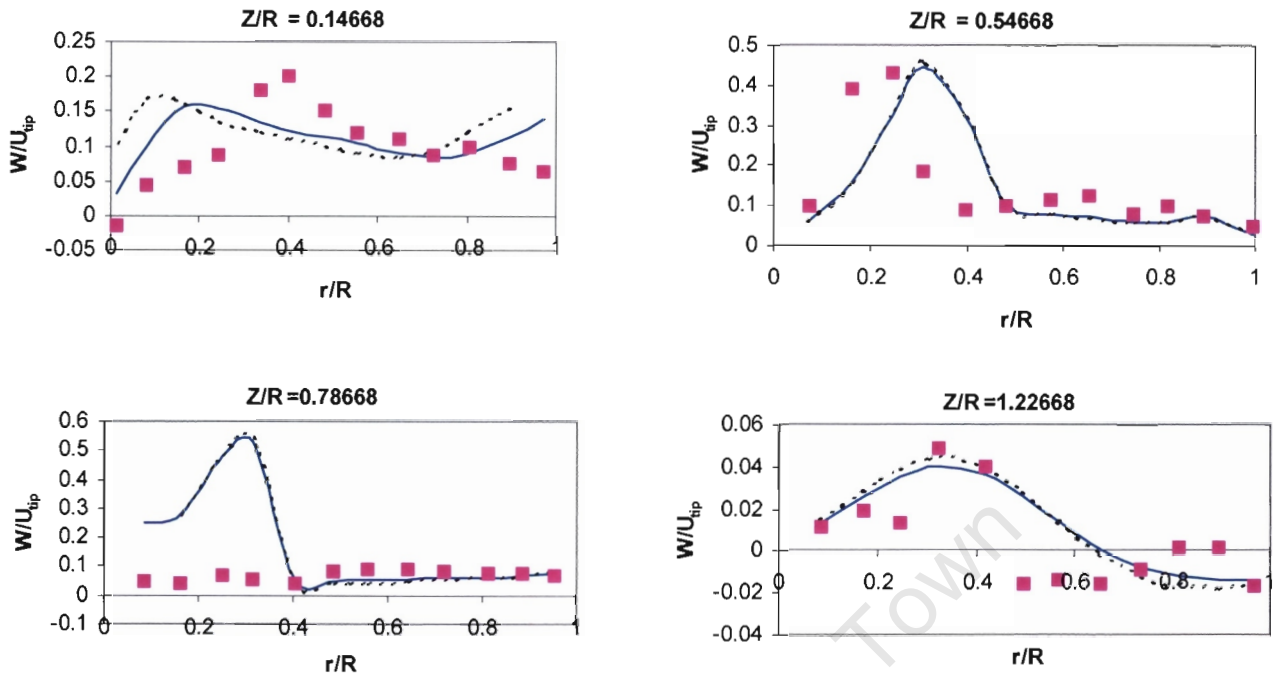


Figure J7: Tangential velocities of 60° pitched blade turbine with model parameters

$C_{\mu}=0.045, C_{\epsilon 1}=1.25, C_{\epsilon 2}=2$: ■ LDA, ---- Standard $k-\epsilon$ model, — Optimum model parameters

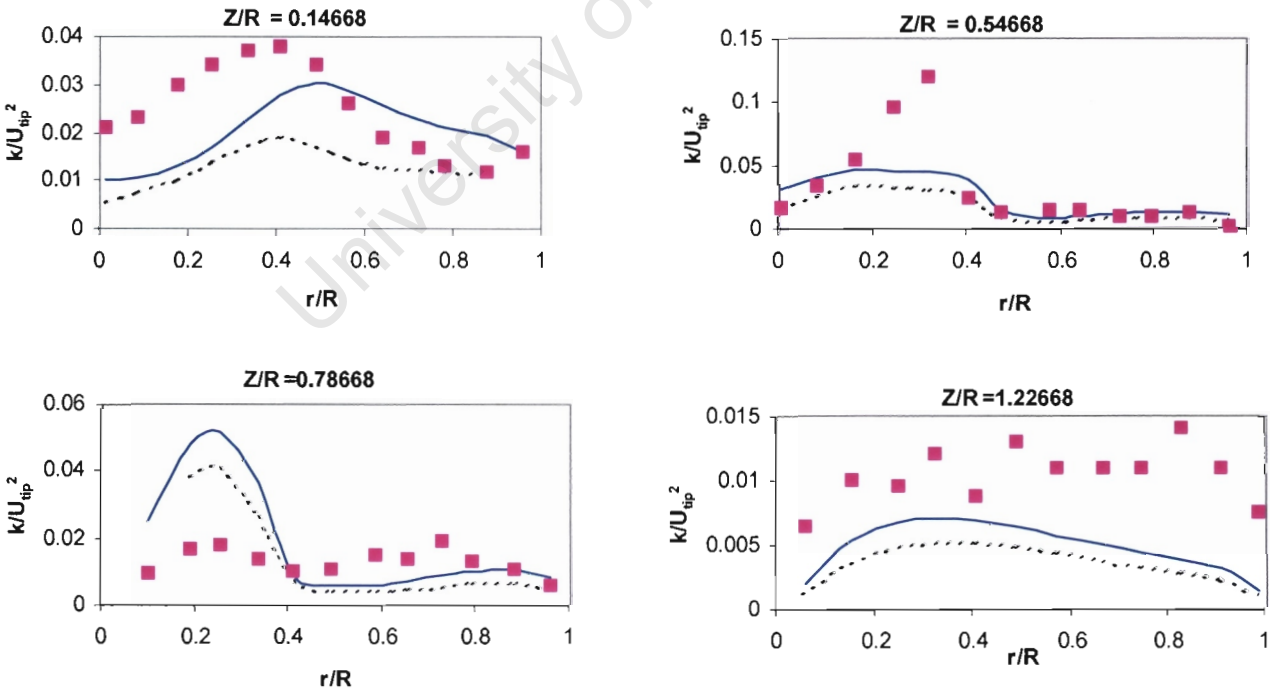


Figure J8: Turbulent kinetic energy of 60° pitched blade turbine with model parameters

$C_{\mu}=0.045, C_{\epsilon 1}=1.25, C_{\epsilon 2}=2$: ■ LDA, ---- Standard $k-\epsilon$ model, — Optimum model parameters

APPENDIX K**Source code for plotting the surface**

```
% Read data from the excel file
data = xlsread('book2.xls');
% extract data
c1=data(:,1); % c1 is in column 1
c2=data(:,2); % c1 is in column 2
z=data(:,3); % error is in column 3

rangeX=floor(min(c1)).01:ceil(max(c1));
rangeY=floor(min(c2)).01:ceil(max(c2));

[X,Y]=meshgrid(rangeX,rangeY);
Z = griddata(c1, c2, z, X, Y,'cubic');
surf(X,Y,Z);

rotate3d;

xlabel('C_\epsilon_1')
ylabel('C_\epsilon_2')
zlabel('Error values')

title('C_\mu = 0.09')
```