

Investigation into the velocity distribution through an annular packed bed

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Dissertation submitted in partial fulfilment of the requirements for the
Masters degree in Mechanical Engineering
at the
School of Mechanical Engineering,
Potchefstroom Campus of the North-West University

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Potchefstroom

2009

Abstract

The purpose of this study was to investigate the velocity distribution through an annular bed packed randomly with equal sized spheres. Extensive research has been conducted on the velocity distribution inside packed beds packed with equal sized spheres, different sized spheres, deformed spheres, cylinders and Raschig-rings. A majority of these experimental and numerical studies focused on the cylindrical packed bed. These studies and numerical models are all confined to the velocity profile once the fluid flow is fully developed. The development of the velocity through the inlet region of the bed and the fluid flow redistribution in the outlet of the bed is thus neglected.

The experimental investigation into the velocity distribution down stream of the annular packed bed of the HTTU indicated that the velocity profile was independent of the mass flow rate for a particle Reynolds number range of $439 \leq Re \leq 3453$. These velocity profiles did not represent the distribution of the axial velocity due to shortcomings associated with the single sensor hot wire anemometry system used to measure the velocity distribution. A numerical investigation, using the RANS CFD code STAR-CCM+[®], into the velocity distribution downstream of an explicitly modelled bed of spheres indicated that the axial velocity distribution could be extracted from the experimental velocity profiles by using an adjustment factor of 0.801. This adjusted velocity profile was used in the verification of the implicit bed simulation model.

The implicit bed simulation model was developed in STAR-CCM+[®]. The resistance of the spheres was modelled using the KTA (1981) pressure drop correlation and the structure of the bed was modelled using the porosity correlation proposed by Martin (1978), while the effective viscosity model of Giese *et al.* (1998), adjusted by a factor of 0.8, was used to model the velocity distribution in the near wall region. It was found that the structure in the inlet region of the bed, where two walls disturb the packing structure, can be modelled as the weighted average of the radial and axial porosity while the structure in the outlet regions can be modelled by letting the radial porosity increase linearly to unity.

The basic shape of the velocity profile is established immediately when the fluid enters the bed. The amplitude of the velocity peaks however increase in magnitude until the velocity profile is fully developed at a distance approximately of five sphere diameters from the bed inlet. The profile remains constant throughout the bed until the outlet region of the bed is reached. In the outlet region a significant amount of fluid redistribution is observed. The amplitude of the velocity peaks is reduced and the position of the velocity peaks is shifted inwards towards the centre of the annular region.

The fully developed velocity profile, predicted by the simulation model is in good agreement with profiles presented by amongst others Giese *et al.* (1998). The current model however also offers insight into the

development of the profile through the inlet of the bed and the fluid redistribution, which occurs in the outlet region of the bed.

Keywords: Randomly packed annular bed, Velocity distribution, Pressure drop, Effective viscosity, Porosity, RANS, CFD, STAR-CCM+[®]

Opsomming

Die doel van die ondersoek was om die snelheidsverdeling deur 'n annulêre bed, willekeurig gepak met sferes, te ondersoek. 'n Beduidende hoeveelheid navorsing is reeds gedoen rakende die snelheidsverdeling deur 'n bed gepak met sferes van gelyke groottes, variërende groottes, vervormde sferes, silinders en Raschig-ringe. Die meerderheid van die eksperimentele en numeriese studies is egter beperk tot silindriese beddens en ondersoek slegs die snelheidsprofiel op 'n afstand binne die bed waar die vloeier ten volle ontwikkel is. Die ontwikkeling van die vloeiveld by die inlaat van die bed en die vloeier herverdeling by die uitlaat van die bed word egter uitgesluit uit die studies.

Die eksperimentele ondersoek na die snelheidsverdeling stroom-af van die annulêre bed van die HTTU het getoon dat die snelheidsprofiel onafhanklik is van die massavloeier deur die bed vir 'n partikel Reynolds-getalreeks van $439 \leq Re \leq 3453$. Die snelheidsprofile het egter nie die verdeling van die aksiale snelheidskomponent verteenwoordig nie, weens tekortkominge verbonde aan die enkelsensor-warmdraad anemometerstelsel wat gebruik was gedurende die snelheidsmetings. Tydens 'n numeriese ondersoek na die vloeiverdeling bo 'n aantal eksplisiet gemodelleerde sferes is daar gevind dat die aksiale snelheidsverdeling vanuit die gemete snelheidsprofile kan onttrek word deur gebruik te maak van 'n aanpassingsfaktor van 0.801. Die aangepaste/aksiale snelheidsprofiel is gebruik in die verifikasie van die implisiete bedsimulasiemodel.

Die implisiete bedsimulasiemodel is ontwikkel in die RANS CFD sagtewarepakket STAR-CCM+®. Die weerstand van die sferes is beskryf m.b.v. die KTA-drukvalvergelyking (1981) terwyl die struktuur van die bed beskryf is m.b.v. die porositeitkorrelasie van Martin (1978). Die na-wandvloeigebied is d.m.v. Giese *et al.* (1998) se effektiewe viskositeitkorrelasie beskryf wat aangepas is met 'n faktor van 0.8 om beter ooreenstemming tussen die aangepaste en gesimuleerde snelheidsprofile te verkry. Daar is gevind dat die struktuur in die inlaatgebied van die bed, waar twee wande die pakkingstruktuur versteur, die beste benader kan word as 'n geweegde gemiddelde van die aksiale en radiale porositeite, terwyl die struktuur in die uitlaatgebied van die bed benader kan word deur die radiale porositeit liniêr te laat toeneem tot een.

Die basiese vorm van die snelheidsprofiel word oombliklik daargestel sodra die vloeier die bed binnedring. Die amplitude van die snelheidspieke neem egter nog in grootte toe totdat die vloeiverdeling ten volle ontwikkel is. Die snelheidsprofiel bereik 'n gestadigde vorm op 'n afstand van nagenoeg vyf sferediameters vanaf die inlaat van die bed. Die snelheidsprofiel bly dan konstant regdeur die bed totdat die vloeier die uitlaatgebied van die bed binnedring. In die gebied geskied daar 'n aansienlike hoeveelheid vloeiherverdeling. Die amplitude van die snelheidspieke neem af in grootte en die pieke word inwaarts verskuif na die middel van die annulêre gebied.

Die ten volle ontwikkelde snelheidsprofiel, wat deur die model voorspel word, toon goeie ooreenstemming met snelheidsprofile wat deur ander navorsers (Giese *et al.*, 1998) gepubliseer is. Die huidige model verskaf egter

ook inligting rakende die ontwikkeling van die snelheidsprofiel in die inlaatgebied van die bed asook die vloeiherverdeling wat plaasvind in die uitlaatgebied van die bed wat voorheen geïgnoreer was.

Kernwoorde: Willekeurige gepakte annulêre bed, Snelheidsverdeling, Drukval, Effektiewe viskositeit, Porositeit, RANS, CFD, STAR-CCM+[®]

Acknowledgements/Bedankings

Eerstens alle lof en eer aan my Hemelse Vader wat my ryklik geseën het met die verstand, krag en deursettingsvermoë om die studie te kon uitvoer.

Baie dankie aan my studieleier, Professor Jat du Toit, en mede-studieleier, Meneer Willem van Niekerk, wat hierdie onderwerp aan my voorgestel het en altyd beskikbaar was om leiding te bied.

'n Spesiale woord van dank aan M-Tech Industrial (PTY.) LTD. en PBMR (PTY.) LTD. wat my toegelaat het om hul toetsfasiliteite en toetsdata te kon gebruik.

Baie dankie aan my familie en vriende wat altyd daar was om my aan te spoor, te motiveer en te ondersteun tydens die verloop van die studie.

Laastens wil ek THRIP bedank sonder wie se befondsing die studie nie uitgevoer sou kon word nie.

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Nomenclature

Latin – Lowercase

<i>Symbol</i>	<i>Description</i>	<i>Unit</i>
d	Diameter	m
f_1	factor in extended Brinkman equation	$\text{kg/s} \cdot \text{m}^3$
f_2	factor in extended Brinkman equation	kg/m^4
f	source term	$\text{kg/m}^2 \cdot \text{s}^2$
h	convection heat transfer coefficient	$\text{W/m}^2 \cdot \text{K}$
k	conduction heat transfer coefficient	$\text{W/m} \cdot \text{K}$
m	distance from bed support wall	m
n	constant in heat loss equation	-
n	number of readings	-
n	distance from container wall	m
p	pitch between spheres	m
r	Radial	-
r	Radius	m
x	parameter in radial porosity distribution correlation	-
x	parameter in velocity profile correlation	-
x	position	m
y	parameter in radial axial porosity distribution correlation	-
z	Axial	-

Latin – Uppercase

<i>Symbol</i>	<i>Description</i>	<i>Unit</i>
A	constant in friction factor	-
A	constant in heat loss equation	-
A	constant in velocity calibration curve	-
A	Area	m^2
B	constant in friction factor	-
B	heat loss equation	-
B	constant in velocity calibration curve	-
C	constant in porosity correlation	-
C	constant in velocity calibration curve	-
C	cell size	m
D	Diameter	m
D	constant in velocity calibration curve	-

E	constant in effective viscosity correlation	-
E	constant in velocity calibration curve	-
E	CTA bridge voltage	V
F	constant in effective viscosity correlation	-
F	constant in velocity calibration curve	-
G	constant in effective viscosity correlation	-
I	Current	A
L	bed length	m
N	constant in porosity correlation	-
P	Pressure	Pa
Q	heat loss	W
R	Radius	m
R	resistance – electric	ohm
R	porous resistance	kg/m ³ · s
T	Temperature	°C
U	Uncertainty	m/s
V	Velocity	m/s
W	Power	Watt

Greek

<i>Symbol</i>	<i>Description</i>	<i>Unit</i>
Δ	Difference	-
ε	Porosity	-
μ	Viscosity	Pa · s
θ	Tangential	-
ρ	Density	kg/m ³
γ	particle diameter to inner cylinder radius ratio (d_p / R_i)	-
ω	constant in effective viscosity correlation	rad
ψ	friction factor	-

Dimensionless Numbers

<i>Symbol</i>	<i>Description</i>
Nu	Nusselt number
Re	Reynolds number

Subscripts

<i>Symbol</i>	<i>Description</i>	<i>Symbol</i>	<i>Description</i>
0	overheat adjustment	max	maximum
0	infinite bed	min	minimum
0	Superficial	<i>ncm</i>	no contact modification
<i>a</i>	Ambient	<i>o</i>	outer
<i>b</i>	Bulk	<i>p</i>	particle
<i>cal</i>	Calibration	<i>p</i>	point
<i>calc</i>	Calculated	<i>r</i>	radial component
<i>cm</i>	contact modification	<i>reslt</i>	resultant
<i>cont</i>	Contact	<i>s</i>	size
<i>corr</i>	Corrected	<i>s</i>	simulated
<i>drift</i>	Drift	<i>stdev</i>	standard deviation
<i>eff</i>	Effective	<i>t</i>	tube
<i>f</i>	Dynamic	<i>tar</i>	target
<i>f</i>	Fluid	<i>x</i>	x component
<i>h</i>	Hydraulic	<i>y</i>	y component
<i>i</i>	Inner	<i>z</i>	z component
<i>i</i>	i th reading	<i>z</i>	axial component
<i>i</i>	Inertial	<i>v</i>	viscous
inter	Interstitial	<i>w</i>	Wall
<i>inst</i>	Instrument	<i>w</i>	wire
<i>m</i>	Modified	θ	tangential component
<i>m</i>	Measured		

Mathematical

<i>Symbol</i>	<i>Description</i>
$\vec{}$	Vector
$\bar{}$	Average

Abbreviations

CFD	Computational Fluid Dynamics
CTA	Constant Temperature Anemometry
DNS	Direct Numerical Simulation
HPTU	High Pressure Test Unit
HTR	High Temperature Reactor

HTTF	Heat Transfer Test Facility
HTTU	High Temperature Test Unit
KTA	Kern Technisches Ausschuss
LBM	Lattice Boltzman Method
LDA	Laser Doppler Anemometry
LDV	Laser Doppler Velocimetry
LES	Large Eddy Simulation
MRI	Magnetic Resonance Imaging
NMR	Nuclear Magnetic Resonance
PIV	Particle Image Velocimetry
RANS	Reynolds-Averaged Navier-Stokes
PBMR	Pebble Bed Modular Reactor

Chapter 1

Introduction

1.1 Introduction

The velocity distribution through a packed bed is of great importance in the design of thermal and mass transport systems (Price, 1968: 7). The applications of packed beds, in these thermal-fluid systems, include chemical reactors, heat exchangers, fusion reactors blankets and nuclear particle-bed reactors (Mueller, 1999:2458). In order to predict the thermal-fluid performance of these systems it is essential to know the pressure drop and velocity distribution through these packed beds. In nuclear packed bed reactors it is essential to be able to predict the maximum fuel temperature and thermal capacitance of the pebble bed core (Rousseau and Van Staden, 2006:1). To be able to predict the thermal-fluid performance of these reactors, the following heat transfer and fluid flow phenomena, existing in these packed beds, must be considered (Rousseau and Van Staden, 2006:1):

- pebble to pebble effective thermal conductivity,
- pebble to reflector effective thermal conductivity,
- pebble to pebble radiation heat transfer coefficient,
- pebble to reflector radiation heat transfer coefficient,
- total pressure drop due to the presence of the pebble bed,
- pebble surface to fluid convection heat transfer coefficient,
- reflector surface to fluid convection heat transfer coefficient and
- effective fluid thermal conductivity due to turbulent mixing.

In the design of the Pebble Bed Modular Reactor (PBMR) various codes such as STAR-CD®, Fluent®, Flownex® and TINTe® are used to predict the PBMR's thermal fluid performance (Rousseau and Van Staden, 2006:1). In modelling the heat transfer and fluid flow phenomena, inside the pebble bed, various thermal-fluid correlations are implemented into these codes. Different simulation methodologies, regarding the implementation of these correlations into an integrated model of the entire pebble, are used in the various codes. A good understanding of the different phenomena along with the manner in which the associated correlations may be implemented is thus required (Rousseau and Van Staden, 2006:1). For this reason PBMR (Pty.) Ltd. commissioned the construction of the Heat Transfer Test Facility (HTTF) that consists of the High Pressure Test Unit (HPTU) and the High Temperature Test Unit (HTTU). The purpose of the HTTF, according to Rousseau and Van Staden (2006:1), is thus twofold:

- The validation of advanced models of the heat transfer and fluid flow phenomena used in the integrated simulation of the pebble bed core via a set of separate effects test.

- To generate results that may be used to validate the different simulation methodologies applied to the integrated modelling of the pebble bed via a set of integrated effects tests.

1.2 Problem Statement

In order to predict the thermal-fluid performance of the HTTU's and PBMR's packed beds the velocity distribution through these packed beds is thus required. Various simulation models and numerical correlations have been developed for the prediction of the flow distribution through various types of packed beds (cylindrical, annular and rectangular). These models only describe the velocity distribution at a distance inside the packed bed where it is presumed that the fluid flow is fully developed. They do not provide any information on the development of the velocity distribution in the inlet and outlet regions of the packed bed.

1.3 Objectives of this study

The purpose of this study is to determine the velocity distribution through the annular packed bed of the HTTU. The study will comprise of both a theoretical and practical investigation into the velocity distribution inside the packed bed.

The practical part of the study will comprise of assisting in the set-up and execution of the velocity tests of the HTTU. These velocity measurements will be made outside the packed bed and will be used in the verification of the model predicting the velocity distribution inside the packed bed. Certain aspects to be carried out include:

- Calibration of the hot wire anemometers and correcting velocity values for variations in temperature;
- Identifying key regions of interest in the flow field;
- Assisting in the execution of the velocity tests;
- Data reduction into presentable velocity profiles;
- Instrument maintenance which include instrument re-calibration and instrument drift calculations; and
- Uncertainty analysis regarding the acquired velocity measurements.

The theoretical part of the study will comprise of the numerical simulation of the velocity distribution through the annular packed bed. The models will be developed with the aid of the commercial Reynolds-Averaged – Navier-Stokes (RANS) computational fluid dynamics (CFD) code and will include:

- an explicit bed simulation model and
- an implicit bed simulation model.

1.4 Outline of this thesis

Chapter 2 presents a literature study of factors influencing the velocity distribution inside packed beds, simulation models (implicit and explicit) of packed beds and velocity measurement techniques. Various correlations and models, used in the simulation of packed beds, are also discussed along with their applicability to the HTTU's pebble bed.

Chapter 3 gives an overview of the method followed in the set-up and execution of the velocity test. Key issues such as the instrument calibration, maintenance and uncertainty regarding the measured velocity profile are discussed.

Chapter 4 discusses the explicit model of a section of a randomly packed bed of spheres used to derive a correlation between the measured velocity and the axial velocity component. The chapter also describes the manner in which the contact points between touching spheres can be treated in cases where heat transfer can be neglected.

Chapter 5 focuses on the development of an implicit model capable of predicting the velocity distribution inside a packed bed. The model builds on the models of previous researchers and is extended to predict the velocity distribution development in the in- and outlet regions of the pebble bed.

Chapter 6 of the dissertation provides an executive summary of the study, concluding remarks and suggestions for future work.

Chapter 2

Literature Survey

2.1 Introduction

The fluid flow through packed beds is of great importance in the development of packed bed thermal-fluid systems such as nuclear reactors and has been extensively researched. The chapter starts off by identifying the various factors influencing the velocity distribution inside a packed bed. An overview of the two methodologies, used in the modelling of packed beds, is also given along with the empirical correlations and models used in the simulation process. The chapter also discusses the different measurement techniques used in the experimental investigation into the velocity distribution inside and downstream of the bed. The chapter concludes with remarks regarding which methodology, correlations, models and measurement technique are most suited to the HTTU's packed bed.

2.2 Factors influencing the velocity distribution

The velocity distribution through a randomly packed bed depends on the following aspects of the bed and the fluid flow through the packed bed:

- the Reynolds number,
- the porosity distribution of the bed,
- particle diameter to cylinder diameter ratio, and
- the length of the bed.

Where the Reynolds number is based on the diameter of the particle and defined as:

$$\text{Re} = \frac{\rho V_0 d_p}{\mu_f} \quad (2.1)$$

with ρ the density of the fluid, V_0 the superficial velocity, d_p the diameter of the particle and μ_f the dynamic viscosity of the fluid. In all further investigations a particle diameter of 60mm will be employed.

Packed beds act like a porous medium, but in contrast to porous media such as sponges, which have a uniform porosity distribution, the porosity in packed beds vary sharply in the near-wall regions. This is due to the fact that the packing structure of the pebbles, at the container wall, deviates from the packing structure in the bulk of the bed. Since an increase in porosity causes the permeability of the porous medium to increase, the velocity distribution is accordingly distorted with higher velocities residing in the near-wall regions of the bed. This is

known as the wall channelling phenomenon (White & Tien, 1987:291). Figure 2-1 illustrates the effect of the wall on the packing structure and the influence of the variation in porosity on the velocity distribution.

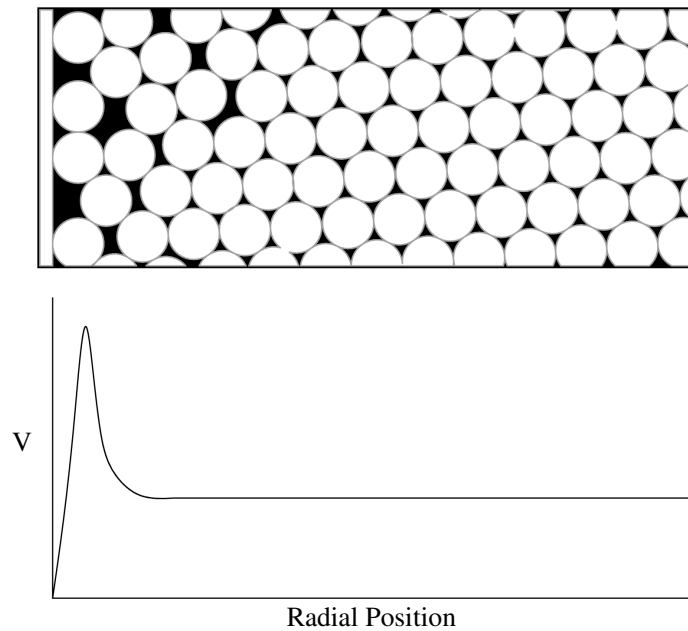


Figure 2-1: Schematic presentation of packing structure and velocity distribution due to wall interface

Price (1968:10) investigated the influence of the flow rate, through the bed, on the velocity distribution experimentally. He found that the normalized velocity distribution is independent of flow rate and accordingly independent of the Reynolds number for ranges $1470 < Re < 4350$. Subagyo *et al.* (1997:1383) developed a new theoretical model for the velocity distribution in packed beds. The model was validated using measurements of velocity made inside and downstream of packed beds. From the results they concluded that for low Reynolds numbers ($Re < 500$) the velocity distribution is dependent on the Reynolds numbers. For Reynolds numbers larger than 500, the velocity distribution's dependency on the Reynolds number is no longer significant. The results of Subagyo *et al.* (1997:1383), indicating the dependency of the velocity distribution on the Reynolds number, is shown in Figure 2-2.

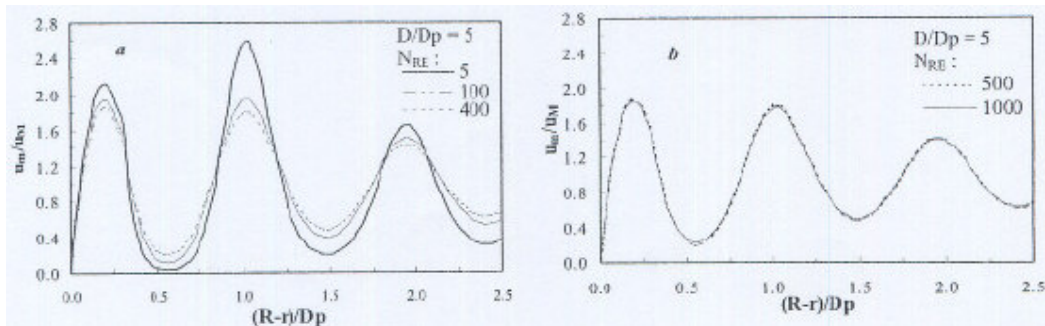


Figure 2-2: The effect of the Reynolds number on the velocity distribution inside a bed of spherical particles for low (a) and high (b) ranges (Subagyo *et al.*, 1997:1383)

Giese *et al.* (1998) conducted similar experimental and theoretical investigations. Giese *et al.* (1998:484) measured the velocity distribution inside a cylindrical packed bed with a cylinder diameter to particle diameter ratio of $D_t / d_p = 9.3$ for Reynolds number ranges of $4 \leq Re \leq 532$. Giese *et al.* (1998:487) noted the same dependency on Reynolds numbers. In their published results only minor distinctions could be made between the profiles at a Reynolds numbers of 103 and 532. The predicted and measured flow distribution inside a bed of spheres at various Reynolds numbers of Giese *et al.* (1998:487) are shown in Figure 2-3.

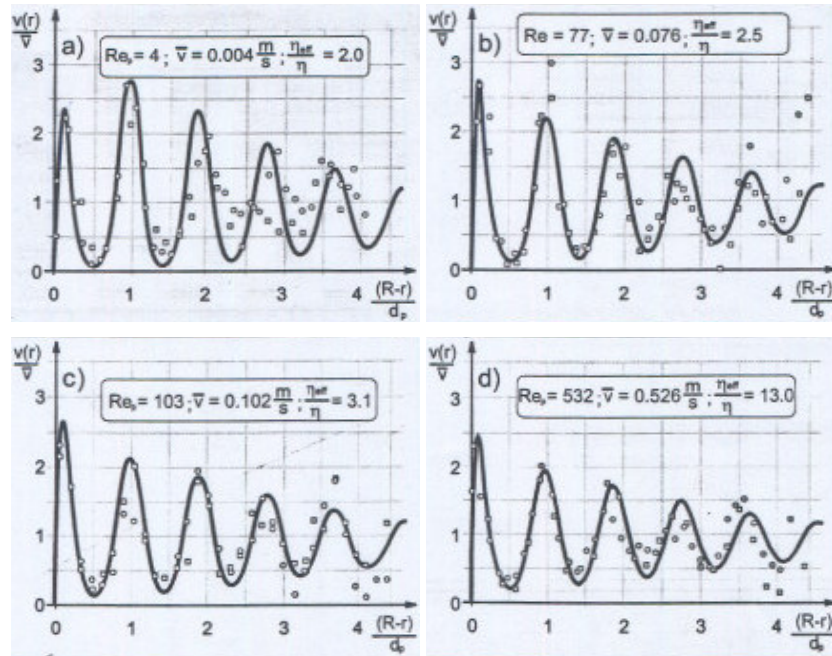


Figure 2-3: Simulated (full line) and experimental flow distributions within a bed of spheres at Reynolds numbers of 4 (a), 77 (b), 103 (c) and 532 (d) (Giese *et al.*, 1998:487)

From these results a larger secondary peak in the velocity distribution can be expected for very low flow rates corresponding to Reynolds numbers smaller than 5. For Reynolds numbers larger than 5, the shape of the velocity profile seems to remain identical while the amplitude of the oscillations decrease slightly. The flow distribution inside the packed bed is independent of the flow rate through the bed for Reynolds numbers larger than 500.

Cheng and Hsu (1986:1843) investigated the velocity distribution through an annular packed bed under forced convective flow with wall effects theoretically. To investigate the influence of the particle diameter on the velocity distribution, three different particle diameters were employed in the simulation model. In order to quantify their results they introduced a dimensionless variable (γ) that is the particle diameter to inner cylinder radius ratio (Cheng & Hsu, 1986:1845). The dependency of the velocity distribution and the wall effect on the particle diameter is shown in Figure 2-4.

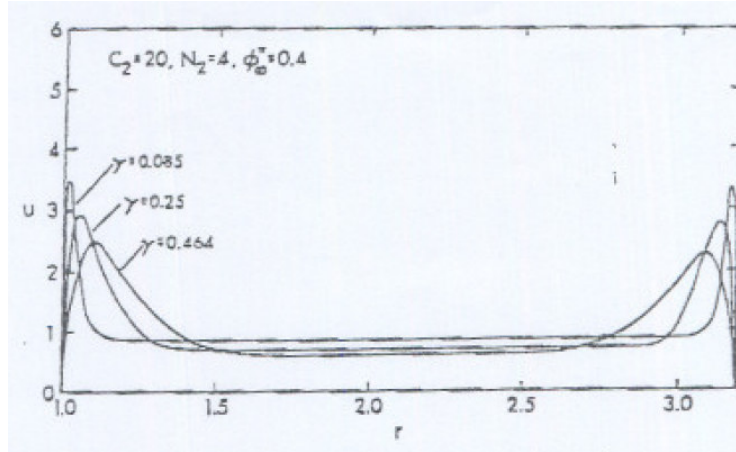


Figure 2-4: Wall channelling effect on axial position (Cheng & Hsu, 1986:1848)

The velocity peaks, in the near-wall regions of the bed, increases as the γ decreases. A higher velocity peak will thus result when using particles with smaller diameters. The velocity peak near the inner wall is also slightly higher than the peak at the outer wall of the annulus. At the inner wall, the maximum velocity is observed at a distance of approximately a quarter particle diameter from the wall and at the outer wall the distance, the corresponding peak velocity is about a third of a particle diameter (Cheng & Hsu, 1986:1843) from the wall.

The depth of the packed bed also influences the velocity distribution through the bed. If the bed was to consist of only a few rows of particles, flow channelling will be observed over the entire bed. A minimum bed length is thus required for the velocity distribution to develop fully. Price (1968:11) investigated the effect of the bed length on the velocity distribution and found the velocity distribution to be independent of the bed length for $L/d_p > 9$.

2.3 Packed bed simulation models

In packed bed simulation models one of two approaches can be followed in the modelling of the structure of the bed (Du Toit, 2008:3074) i.e.

- a discrete approach and
- a continuum approach.

In the discrete approach the spheres and pores of the packing are modelled explicitly where any point $\vec{x}$ is situated either inside a pore or inside a sphere. The porosity at the point is then given as

$$\varepsilon(\vec{x}) = \begin{cases} 0, & \text{for the point inside a sphere} \\ 1, & \text{for the point inside a pore} \end{cases} \quad (2.2)$$

The discrete approach is normally followed when using direct numerical simulations (DNS), large eddy simulations (LES) and lattice Boltzmann methods (LBM). These methods normally require a large amount of resources causing the evaluation domains to be limited in size (Du Toit, 2008:3074).

Alternatively, the pores and spheres can be taken into account implicitly using the continuum approach where the presence of the spheres is modelled implicitly. This approach is most commonly used and employed in Reynolds-averaged Navier-Stokes (RANS) codes (Du Toit, 2008:3074). For a point $\vec{x}$ in the packed bed the porosity is thus given as

$$\varepsilon(\vec{x}) = f(\vec{x}) \text{ with } 0 \leq f(\vec{x}) \leq 1 \quad (2.3)$$

This approach only models the effect of the spheres and does not provide any detail about the flow around the spheres (Du Toit, 2008:3074).

When the continuum approach is used a number of empirical correlations are employed to model the presence of the spheres and the influence the spheres have on the flow distribution inside the bed. The basis of an implicit simulation model is a correlation describing the structure (porosity) of the bed along with a pressure drop correlation, which models the resistance the flow experiences due to the presence of the spheres. Some researchers (Bey & Eigenberger, 1996; Giese *et al.*, 1998; Ziolkowska and Ziolkowski, 1993) found the use of these two correlations insufficient in modelling the velocity distribution inside the bed. Their simulation models predicted velocity distributions with too high velocity peaks in the region near the wall. For this reason they employed an “effective turbulent viscosity” to dampen the velocity peaks in the near wall region in order to achieve a better fit between their simulated and measured velocity profiles.

In using the discrete modelling approach the spheres are modelled explicitly. A large number of studies have been conducted on the fluid flow and heat transfer through packings of discretely modelled spheres using CFD calculations. The spheres in these packings were arranged in either a structured grid (Wang-Kee In & Hassan, 2008; Logtenberg *et al.*, 1999; Nijemeisland & Dixon, 2001; Calis *et al.*, 2001; Guardo *et al.*, 2005; Lee *et al.*, 2007) or were randomly placed spheres (McLaughlin *et al.*, 2008).

These studies contain a variety of model generation techniques. Several issues related specifically to mesh generation have been identified. These include:

- the treatment of sphere-to-spheres and sphere-to-wall contacting points and
- placement of a fine mesh near the sphere surface.

Other issues related to model generation are that of the transition from a laminar to turbulent flow regime and the use of a suitable turbulence model.

In the following sections the correlations and key components of each of these two modelling approaches will be discussed.

2.3.1 Implicit bed simulation models

In this section an overview of the correlations used in the implicit bed modelling approach is provided. The section concludes with an overview of implicit simulation models that have been developed by other researchers.

2.3.1.1 Porosity distribution models

The presence of the container wall in packed beds causes the packing structure of the bed to deviate in these near wall regions. In these regions the packing is less dense than in the core of the bed, causing the porosity of the bed to increase in the vicinity of the wall (Goodling *et al.*, 1982:24).

At the container wall, there is only a point contact between the particles and the wall, which causes the porosity to approach unity as the distance to the container wall is decreased. As one moves away from the wall, the porosity decreases to a minimum at approximately half a particle diameter from the wall. Moving further inward towards the centre of the bed, the porosity starts to increase again until a second peak in porosity is observed at a distance of one particle diameter from the wall. This is the point of maximum porosity for a particle that is not in contact with the container wall. This peak does not approach unity, as seen at the container walls, since the second row of particles rest in the cups formed by the first row of particles, which are in contact with the container wall. This phenomena repeats itself the further one moves away from the container wall. Due to the fact that the randomness of each row increases as the distance from the wall is increased, the porosity oscillates around the bulk porosity (porosity at the centre of the bed) with a decrease in amplitude (Goodling *et al.* 1982:29). For cylindrical packed beds, consisting of uniformly sized spheres, this oscillation in porosity can be detected as far as five sphere diameters from the containing wall (Goodling *et al.* 1982:23).

This variation in porosity causes the velocity profile to be distorted accordingly, with the velocity reaching a maximum in the near-wall region of the packed bed (Du Toit, 2008:3073). This phenomenon is known as wall channelling and may have a significant impact on the heat and mass transfer in the bed (Hunt & Tien, 1987:291). As a result, a proper understanding of the porosity distribution is required in order to analyse the transport phenomena in a packed bed (Goodling *et al.*, 1982:23).

Various empirical correlations to describe the radial variation in porosity have been proposed by different researchers. These correlations can be divided into two categories namely exponential and damped oscillatory correlations. The damped oscillatory correlations attempt to describe the oscillatory behaviour of the variation in porosity while the exponential correlations attempt to describe the variation of the average porosity.

Du Toit (2008:3078) considered a number of exponential correlations and found that the correlation proposed by Hunt & Tien (1990:57) provided the best prediction of average variation in the core of the heat transfer test facility (HTTF). Following Cheng and Hsu (1986:1845) and Sodré and Parise (1998:267) the radial variation in porosity for an annular packed bed can be written as

$$\varepsilon(r) = \varepsilon_0 \left[1 + C \exp \left(-N \frac{r - R_i}{d_p} \right) \right] \quad \text{for } R_i \leq r \leq \frac{R_o - R_i}{2} \quad (2.4)$$

$$\varepsilon(r) = \varepsilon_0 \left[1 + C \exp \left(-N \frac{R_o - r}{d_p} \right) \right] \quad \text{for } \frac{R_o - R_i}{2} \leq r \leq R_o \quad (2.5)$$

with ε_0 the porosity of an infinite bed (bed with no walls), R_i is the inner annulus radius, R_o is the outer annulus radius, r the radius at which the porosity is to be determined and C and N are constants.

Hunt and Tien (1990:57) took $\varepsilon_0 = \varepsilon_b$ the bulk porosity of the bed. They also took the value of N to be $N = 6$ for perfectly spherical particles. The value of C is calculated so that (2.4) and (2.5) yields a porosity of 1 at the annulus walls.

Du Toit (2008:3077) also considered a number of oscillatory correlations and found that the correlation proposed by Martin (1978: 915) provided the best prediction of the oscillatory variation in the porosity of the HTTF. Martin (1978:915) derived his correlation from the experimental data of Benenati and Brislow (1962) and the porosity distribution through a cylindrical packed bed can be written as

$$\varepsilon(r) = \begin{cases} \varepsilon_{\min} + (1 - \varepsilon_{\min}) x^2 & \text{for } -1 \leq x \leq 0 \\ \varepsilon_b + (\varepsilon_{\min} - \varepsilon_b) e^{\frac{-x}{4}} \cos \left(\frac{\pi}{C} x \right) & \text{for } x \geq 0 \end{cases} \quad (2.6)$$

with

$$x = 2 \frac{R_o - r}{d_p} - 1 \quad (2.7)$$

and

$$C = \begin{cases} 0.816 & \text{for } \frac{D_t}{d_p} = \infty \\ 0.876 & \text{for } \frac{D_t}{d_p} = 20.3 \end{cases} \quad (2.8)$$

where $\varepsilon_{\min}$ is the minimum porosity in the near-wall region and ranges from $\varepsilon_{\min} = 0.20 \rightarrow 0.26$, ε_b the bulk porosity of the bed which is undisturbed by wall effects. R_o is the outer radius of the cylinder, x the dimensionless distance from the wall as defined in equation (2.7), C the dimensionless parameter as defined in equation (2.8) and D_t the diameter of the cylinder.

The results of Du Toit's (2008: 3077) investigation into the oscillatory correlations are shown graphically in Figure 2-5.

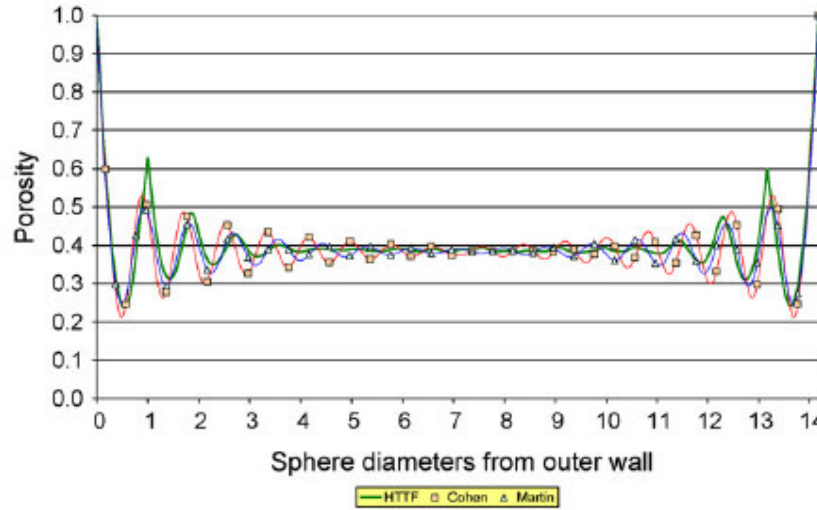


Figure 2-5: Comparison between oscillatory correlations and numerical results for the HTTF (Du Toit, 2008: 3077)

The correlation proposed by Martin (1978: 915) under predicts the second peak in porosity and the velocity profile may be affected accordingly.

In the study conducted by Du Toit (2008) the correlation of De Klerk (2003:2028) was not evaluated. The same exponentially damped sinusoidal form than that of Martin (1978:915) was used by De Klerk (2003) in the development of his model. De Klerk (2003:2028) determined the constants of the model by fitting the form of the correlation to porosity data found in the literature. The constants were then adjusted so that the correlation yielded sensible average bed porosities. The radial variation of porosity through a cylindrical packed bed can be written as

$$\varepsilon(r) = \begin{cases} 2.14x^2 - 2.53x + 1 & \text{for } x \leq 0.637 \\ \varepsilon_b + 0.29e^{-0.6x} \cos(2.3\pi(x-0.16)) + 0.15e^{-0.9x} & \text{for } x > 0.637 \end{cases} \quad (2.9)$$

with

$$x = \frac{R_o - r}{d_p} \quad (2.10)$$

The difference between the porosity predicted by the models of Martin (1978) (2.6) and De Klerk (2008) (2.9) are presented graphically in Figure 2-6.

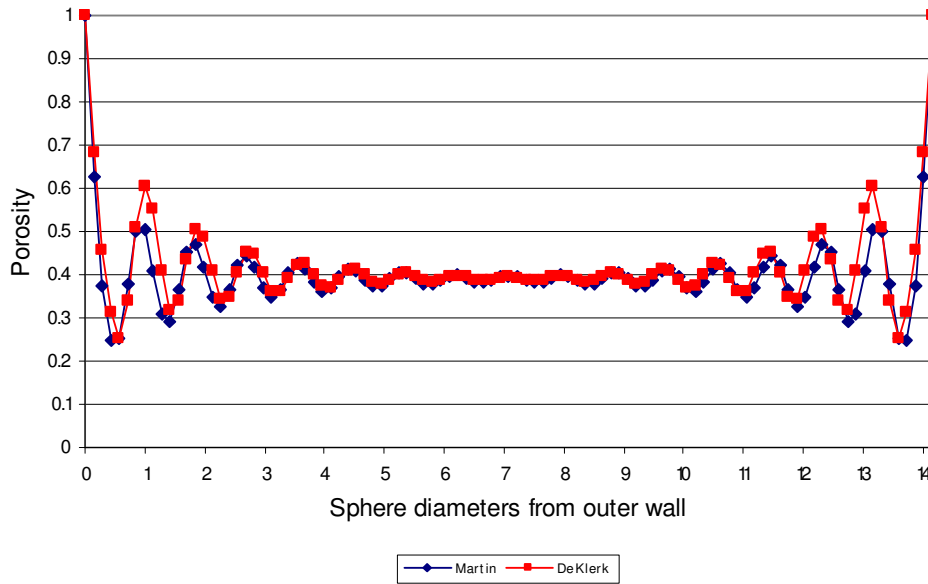


Figure 2-6: Comparison between oscillatory correlations of Martin (1977) and De Klerk (2003)

When comparing the predicted porosity distributions of De Klerk (2003) and Martin (1978), shown in Figure 2-6, with the numerically obtained porosity distribution of the HTTF, shown in Figure 2-5, it will appear as though the correlation proposed by De Klerk (2003) is superior. The correlation of De Klerk (2003) is thus preferred.

It should however be remembered that these correlations only describe the average structure of the bed and give no insight into the actual position of the spheres in the packing. Furthermore, these correlations only describe the radial variation in porosity. They can however be adapted to describe the variation in porosity in the axial direction. Uncertainty, regarding the structure of the bed, still remains in regions where two walls disturb the packing (corners of the packing near the tube and bed support walls) and in the outlet region of the packing.

2.3.1.2 Pressure drop models

Brinkman (1947) as cited by Vortmeyer and Schuster (1983:1692) was the first to formulate the differential equation to describe the flow distribution inside a porous medium bounded by rigid walls. Brinkman (1947) developed his model by extending Darcy's law by a viscous term to account for the viscous forces near the walls (Vortmeyer & Schuster, 1983:1692). The model however only holds true for low flow rates (Vortmeyer & Schuster, 1983:1692).

Ergun (1952:89) developed an empirical correlation to predict the pressure loss per unit bed length of a packed bed. In his investigation he found that the pressure loss is simultaneously caused by both kinetic and viscous energy losses. Ergun (1952) discovered that these energy losses strongly depend on the porosity of the bed, with the viscous energy loss being proportional to $(1-\bar{\varepsilon})^2 / \bar{\varepsilon}^3$ while the kinetic energy loss is proportional to $(1-\bar{\varepsilon}) / \bar{\varepsilon}^3$. In its generic form the pressure drop per unit bed length can be written as:

$$\frac{\Delta P}{\Delta L} = \psi \frac{1-\bar{\varepsilon}}{\bar{\varepsilon}^3} \cdot \frac{1}{d_p} \cdot \frac{\rho V_0^2}{2} \quad (2.11)$$

with ΔP the pressure drop over a bed length ΔL , ψ the friction factor, $\bar{\varepsilon}$ the average porosity of the bed, ρ the density of the fluid and V_0 the superficial velocity through the bed.

Ergun (1952) found that the correlation for the friction factor is:

$$\psi = \frac{300}{\text{Re}_m} + 3.5 \quad (2.12)$$

with

$$\text{Re}_m = \frac{\text{Re}}{(1-\bar{\varepsilon})} \quad (2.13)$$

with Re_m the modified Reynolds number.

The form of the friction factor, as provided in equation (2.12), is known as an Ergun type friction factor, named after Ergun (1952) who proposed the original version. By inserting equation (2.12), (2.13) and (2.1) equation reference goes here into equation (2.11) and expanding the equation the pressure drop through the bed, per unit bed length, can be written as:

$$\frac{\Delta P}{\Delta L} = 150 \frac{(1-\bar{\varepsilon})^2}{\bar{\varepsilon}^3} \cdot \frac{\mu_f V_0}{d_p^2} + 1.75 \frac{(1-\bar{\varepsilon})}{\bar{\varepsilon}^3} \cdot \frac{\rho V_0^2}{d_p} \quad (2.14)$$

In the development of his correlation Ergun (1952:92) mainly focused on a modified Reynolds number range of $Re_m < 10^3$. The application of the Ergun equation to higher modified Reynolds number ranges is thus questionable.

Since the Brinkman equation is only valid for low flow rates, Vortmeyer and Schuster (1983) extended the correlation by means of the Ergun pressure loss relation so that the model can be applied to higher flow rates. This extension gave rise to the so-called extended Brinkman equation. Giese *et al.* (1998) employed the extended Brinkman in their numerical investigation into the velocity distribution inside the bed. The differential form of the extended Brinkman equation, as used by Giese *et al.* (1998), can be written as:

$$\frac{\partial P}{\partial L} = -f_1 V_0 - f_2 V_0^2 + \frac{\mu_{eff}}{r} \cdot \frac{\partial}{\partial r} \left(r \frac{\partial V_0}{\partial r} \right) \quad (2.15)$$

with f_1 and f_2 factors chosen from the Ergun (1952) pressure loss relation and μ_{eff} the effective viscosity.

These factors are defined as:

$$\left. \begin{aligned} f_1 &= 150 \frac{(1-\bar{\varepsilon})^2}{\bar{\varepsilon}^3} \cdot \frac{\mu_f}{d_p^2} \\ f_2 &= 1.75 \frac{(1-\bar{\varepsilon})}{\bar{\varepsilon}^3} \cdot \frac{\rho}{d_p} \end{aligned} \right\} \quad (2.16)$$

The use of 150 and 1.75 as coefficients in both the Ergun and extended Brinkman equations has been controversial and has been adjusted by various researchers to achieve a better fit between their measured and simulated velocity profiles. Vortmeyer and Schuster (1983:1692) applied values of 175 and 1.75 to the extended Brinkman equation. Yu *et al.* (2001:950) employed values of 203 and 1.95 in their investigation of cylindrical beds of uniform spheres. Macdonald *et al.* (1979:206) re-evaluated the coefficients and found that values of 180 and 1.8, for smooth particles, and values of 180 and 4.0, for rough particles, yielded the best results.

A lesser-known form of friction factor used in equation (2.11) is the Carman type friction factor named after Carman (1937) who proposed the original version. The KTA (Kern Technisches Ausschuss – Safety Standards of the Nuclear Safety Standards Commission, KTA 3102.3 1981) friction factor is of the Carman type. The correlation was developed to predict the pressure drop through high temperature reactors (HTR) that use 60 mm spheres. The KTA (1981) friction factor correlation can be written as:

$$\psi = \frac{320}{\text{Re}_m} + \frac{6}{\text{Re}_m^{0.1}} \quad (2.17)$$

This correlation is only valid for a modified Reynolds number range of $1 \leq \text{Re}_m \leq 10^5$ and a average porosity range of $0.36 \leq \bar{\varepsilon} \leq 0.42$.

By inserting equation (2.17) into (2.11) the pressure drop through the bed can be written as:

$$\frac{\Delta P}{\Delta L} = 160 \frac{(1-\bar{\varepsilon})^2}{\bar{\varepsilon}^3} \cdot \frac{\mu_f V_0}{d_p^2} + 3 \frac{(1-\bar{\varepsilon})^{1.1}}{\bar{\varepsilon}^3} \cdot \left(\frac{\mu_f}{\rho V_0 d_p} \right)^{0.1} \cdot \frac{\rho V_0^2}{d_p} \quad (2.18)$$

These friction factors do not account for the influence of the walls on the pressure drop in the bed. Einfeld and Schnitzlein (2001:4321) tried to quantify the influence the walls have on the pressure drop in packed beds. Einfeld and Schnitzlein (2001:4323) evaluated a total of 2391 pressure drop data sets, 1974 of these sets pertaining to spheres. The data sets cover a particle based Reynolds number range of $0.01 \leq \text{Re} \leq 17635$, average porosity range of $0.330 \leq \bar{\varepsilon} \leq 0.882$ and cylinder diameter to particle diameter ratio range of $1.624 \leq D_t / d_p \leq 250$. These data sets were compared with 24 published pressure drop correlations. Einfeld and Schnitzlein (2001:4326) found the most promising correlation representing the data to be the Ergun type friction factor of Reichelt (1972). The friction factor can be written as:

$$\psi = \frac{308 A_w^2}{\text{Re}_m} + \frac{2 A_w}{B_w} \quad (2.19)$$

with A_w and B_w constants defined as:

$$\left. \begin{aligned} A_w &= 1 + \frac{2}{3(D_t / d_p)(1-\bar{\varepsilon})} \\ B_w &= \left[1.15(d_p / D_t)^2 + 0.87 \right]^2 \end{aligned} \right\} \quad (2.20)$$

A comparison between the predicted pressure drop using the friction factors proposed by Ergun (1952), KTA (1981) and Einfeld and Schnitzlein (2001) for a modified Reynolds number range of $1 \leq \text{Re}_m \leq 10^3$ and $10^3 \leq \text{Re}_m \leq 10^5$ can be seen in Figure 2-7 and Figure 2-8. The friction factor proposed by Einfeld and Schnitzlein (2001) is dependant on the cylinder diameter of the packing. To apply the correlation to an annulus,

the cylinder diameter was replaced with either the annulus width ($D_t = R_o - R_i$) or the hydraulic diameter of the annulus ($D_t = D_h = 2(R_o - R_i)$).

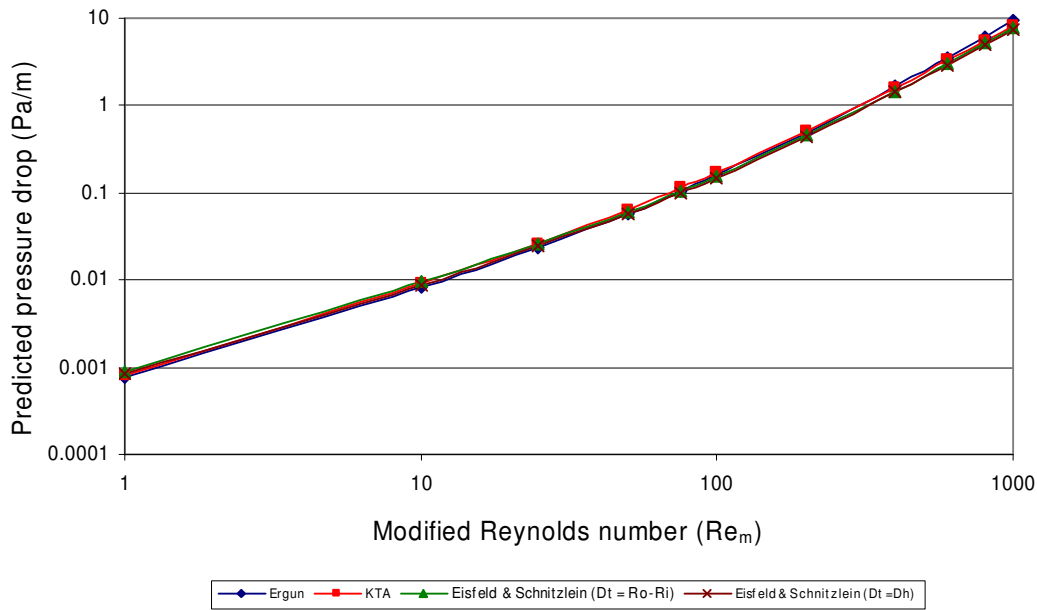


Figure 2-7: Comparison between pressure drop correlations for a modified Reynolds number range of $1 \leq Re_m \leq 10^3$

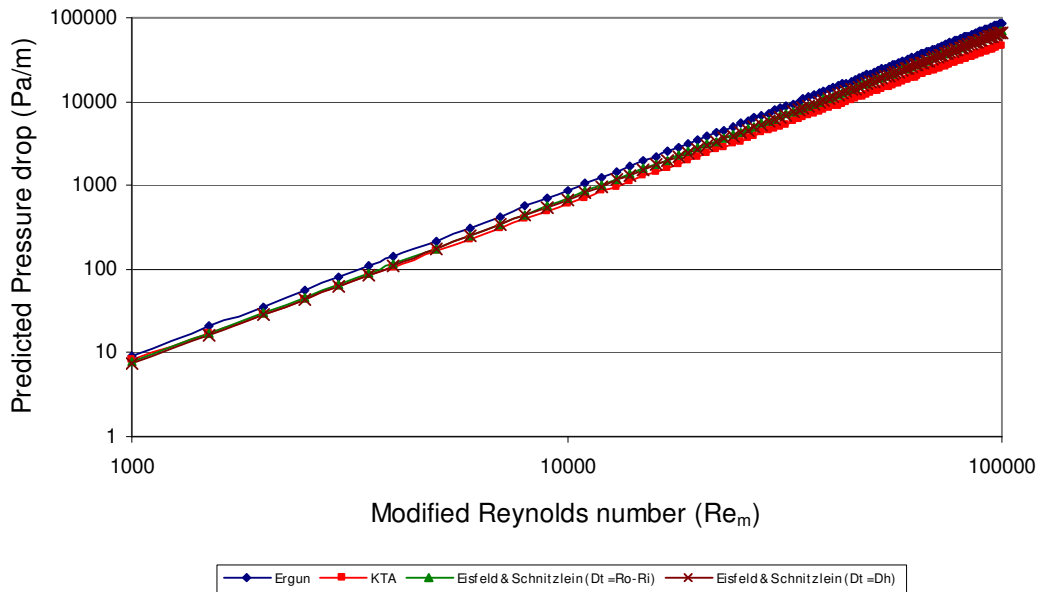


Figure 2-8: Comparison between the pressure drop correlation for a modified Reynolds number range $10^3 \leq Re_m \leq 10^5$

As seen from Figure 2-7 for a modified Reynolds number range of $1 \leq Re_m \leq 1000$ all four friction factors predict pressure drops that are in close agreement with each other. For modified Reynolds numbers larger than 1000 the pressure drop, the prediction of the friction factor proposed by Ergun (1952), starts to deviate strongly

from the pressure drop predicted through the use of the friction factors of Einfeld and Schnitzlein (2001) and KTA (1981). This can be attributed to the fact that the friction factor of Ergun (1952) was developed for modified Reynolds numbers smaller than 1000. The use of this friction factor is thus not recommended for flow conditions corresponding to modified Reynolds numbers larger than 1000. The pressure drop predicted through the use of the KTA (1981) and Einfeld and Schnitzlein's (2001) friction factors are in very close agreement with each other up to a modified Reynolds number of 6000. For modified Reynolds numbers larger than 6000 the friction factor of Einfeld and Schnitzlein (2001) predicts a pressure drop that is higher than that of the KTA (1981) friction factor. This may be because the influence of the walls on the pressure drop becomes more prominent. It is also interesting to note that there is a negligible difference between the pressure drops predicted by the friction factor of Einfeld and Schnitzlein (2001) using the annulus width as the cylinder diameter ($D_t = R_o - R_i$) and the friction factor using the hydraulic diameter of the annulus as the cylinder diameter ($D_t = D_h = 2(R_o - R_i)$).

For modified Reynolds numbers smaller than 1000 any one of the four stated friction factors could be employed. For modified Reynolds numbers smaller than 6000 either the KTA (1981) friction factor or the friction factor of Einfeld and Schnitzlein (2001) can be used.

These friction factors were determined for cylindrically packed beds and their applicability to annular packed beds remains doubtful.

2.3.1.3 Effective viscosity models

It is a well-documented fact that simulation models, based solely on a porosity distribution and pressure drop correlations, as described in the sections above, tend to over predict the velocity peaks in the near wall region. This is due to the fact that the pressure drop correlation is assumed to be valid over the entire porosity range. Bey and Eigenberger (1996:1369) reported a fourfold increase in the wall peak velocity over the mean interstitial velocity inside the packing and that the predicted velocity peaks at the point of measurement were 20% higher than the measured velocities. The use of an "effective turbulent viscosity" to adjust the velocity profile so as to achieve a better fit between the measured and simulated velocity profiles is well documented.

Giese *et al.* (1998:489) conducted an intensive study for a Reynolds number range of $4 \leq Re \leq 532$, on the influence of the effective viscosity on the velocity distribution by incorporating various values for the effective viscosity into their simulation model. Giese *et al.* (1998:489) noted that only the magnitude of the near wall velocity peak was affected, decreasing in magnitude with an increase in effective viscosity while the rest of the velocity profile seemed to remain unaffected. Since the pressure drop correlation is applied to porosities outside the range of the correlation, the porosity in the near wall region has a strong influence on the effective viscosity. Giese *et al.* (1998:448) argued that there exist small fillets of stagnant flow around the contact points

between the spheres and the wall, thus reducing the porosity at the wall. As a matter of interest, Giese *et al.* (1998:448) performed calculations with the wall porosities (ε_w) starting at $\varepsilon_w = 0.8$ and 0.9 instead of one. For these calculations the best fit between the measured and simulated velocity profiles were obtained with $\mu_{eff} / \mu_f = 4$ for $\varepsilon_w = 0.8$ and $\mu_{eff} / \mu_f = 8$ for $\varepsilon_w = 0.9$ instead of $\mu_{eff} / \mu_f = 13$ for $\varepsilon_w = 1$. According to Giese *et al.* (1998:488) the effective viscosity to be employed for spheres can be calculated as follow:

$$\frac{\mu_{eff}}{\mu_f} = 2 \exp(3.5 \times 10^{-3} \text{Re}) \quad (2.21)$$

with μ_{eff} the effective viscosity.

Similarly Bey and Eigenberger (1996:1370) developed their own effective viscosity model. For spheres the best fit between their measured and simulated velocity profiles was achieved with the following correlation:

$$\frac{\mu_{eff}}{\mu_f} = 1 + \left(7 \times 10^{-6} \frac{D_t}{d_p} + 2 \times 10^{-5} \right) \text{Re}^2 \quad (2.22)$$

From the results of Giese *et al.* (1998) it can be argued that no effective viscosity will be needed if the porosity distribution falls inside the region of validity of the pressure drop correlation. Although the effective viscosity only affects the velocity distribution in the near wall region, it can be argued that an effective viscosity correlation is needed that takes the structure of the bed into account rather than applying a constant effective viscosity to the entire bed.

Ziolkowska and Ziolkowski (1993:3290) developed an extensive model for the effective viscosity from their measurements. This model differs from the previous models in that the effective viscosity is not calculated as a single value but is described as a damped oscillatory function reaching a maximum at the walls while the value at the centre of the bed approaches zero. The oscillating effective viscosity for a D_t / d_p range of $10.8 \leq D_t / d_p \leq 22.9$ can thus be calculated as follows:

$$\frac{\mu_{eff}}{\mu_f} = E \left[\exp \left(F \frac{R_o - r}{d_p} \right) \right] \cdot \left[\cos \left(\omega \frac{R_o - r}{d_p} \right) + G \right] \quad (2.23)$$

with

$$\omega = 2.055\pi \quad (2.24)$$

$$G = 0.45 \quad (2.25)$$

$$E = 3.419 - 0.148 \frac{D_t}{d_p} + 0.011 \left(\frac{D_t}{d_p} \right)^2 \quad (2.26)$$

$$F = -0.668 + 0.048 \frac{D_t}{d_p} + 0.004 \left(\frac{D_t}{d_p} \right)^2 \quad (2.27)$$

This correlation however yields somewhat unrealistic effective viscosity values close to the wall and the hydraulic diameter to particle diameter of the HTTU falls just outside the range for which the correlation is valid. Because of this the correlations proposed by Giese *et al.* (1998:489) or Bey and Eigenberger (1996:1370) should rather be used. These correlations also yield unrealistic effective viscosity values when they are applied at higher flow rates.

Du Toit *et al.* (2008:3) determined the effective viscosity for annular packed beds with wall effects numerically. Du Toit *et al.* (2008:5) defined a cylindrical packed bed with the same hydraulic diameter to particle diameter ratio as the annulus width to particle diameter ratio of an annular packed bed $(D_h / d_p = D_t / d_p = (R_o - R_i) / d_p)$. For a specific Reynolds number the pressure gradient was determined for plug flow using the friction resistance correlation proposed by Reichelt (1972) with the coefficients proposed by Einfeld and Schnitzlein (2001:4326). Next Du Toit *et al.* (2008:4) solved the extended Brinkman equation employed by Vortmeyer and Schuster (1983), as adapted by Bey and Eigenberger (1997), Giese *et al.* (1998) iteratively using equation (2.19), using an infinite bed $(d_p / D_t \approx 0)$, for the effective viscosity until the same pressure gradient was obtained. No correlation is given but the data from the study is given bellow in Table 2-1.

Table 2-1: Effective viscosity as a function of Reynolds Number (Du Toit *et al.* 2008:5)

Re	μ_{eff} / μ_f
1000	22.48
2000	42.27
5000	101.67
10000	200.71
20000	398.78
30000	596.87

By fitting a line through the data the effective viscosity as a function of Reynolds number can be written as

$$\frac{\mu_{eff}}{\mu_f} = 0.01981 \text{Re} + 2.652 \quad (2.28)$$

For low Reynolds numbers either the effective viscosity model of Giese *et al.* (1998) or Ziolkowska and Ziolkowski (1993) can be used. For higher flow rates its best to use (2.28) since the models of Giese *et al.*

(1998) and Ziolkowska and Ziolkowski (1993) yield unrealistic effective viscosity values. The need still remains for a model that takes the structure of the bed into account.

2.3.1.4 Temperature influence

Even though the velocity tests were conducted under isothermal fluid flow conditions, the improper treatment of temperature gradients in the simulation model can adversely affect the simulated velocity distribution.

The accuracy of the simulation model depends strongly on the simulation approach being employed. Malan *et al.* state (2004:4) that two possible approaches can be followed to model the conservation of energy; i.e.

- the local-thermal-equilibrium formulation and
- the local-thermal-non-equilibrium formulation.

The first formulation typically entails the employment of a single energy conservation equation for the fluid and particles. This approach has been applied to model high pressure packed bed reactors (Malan *et al.*, 2004:4). Verkerk (2000:23) found this formulation to be only valid in cases when the heat production from the fuel pebbles is low, resulting in low temperature gradients across the bed. This case corresponds to a scrambled reactor and this formulation is not adequate when operational transients are important. The local-thermal-non-equilibrium approach does not suffer from these over-simplifications and is adequate to simulate operational transients (Gunn *et al.* as cited by Malan *et al.*, 2004:4).

Bortolozzi and Deiber (2000:157) investigated the difference between the one-field (local-thermal-equilibrium) and the two-field (local-thermal-non-equilibrium) models to simulate the temperature distribution through an annular packed bed subjected to natural convective flow. The interaction between the fluid and particles were modelled by means of the momentum exchange between the fluid and particles. A coefficient of 180 was assigned to the permeability function and 1.8 to the empirical Forcheimer factor, rather than 150 and 1.75 as in the Ergun equation (Bortolozzi & Deiber, 2000:161). The resulting conservation equations were solved by means of the finite difference method from which the two-dimensional temperature and flow distribution, inside the packed bed, were obtained. The porosity distribution was modelled by means of an exponentially decaying correlation but they also proposed a correlation that accounts for the oscillatory damped variation in porosity. The difference between the velocity distributions obtained from both the one- and two-field models are shown in Figure 2-9.

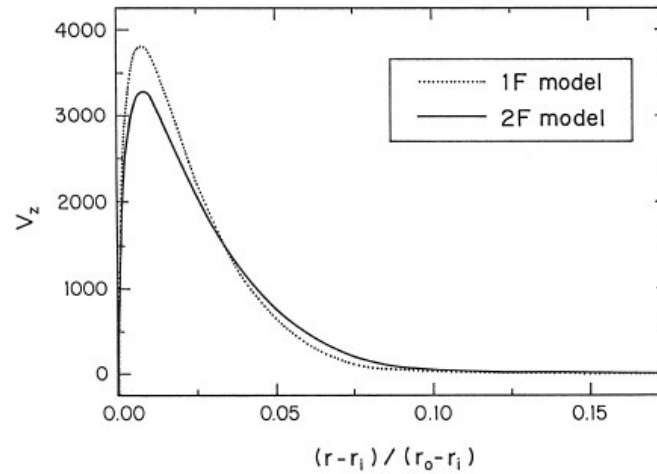


Figure 2-9: Dimensionless velocity V_z near the hot wall at the mid-height of the porous cavity, obtained from 1- and 2-F models, as a function $(r-r_i)/(r_o-r_i)$ (Bortolozzi & Deiber, 2000:166).

The difference in these profiles can be attributed to the fact that the fluid and solid temperature distributions are not the same in the two models and the effect this has on the buoyancy force driving the fluid flow through the packed bed (Bortolozzi & Deiber, 2000:167). When the solid and fluid temperatures are almost identical or close to one another, the velocity profiles from both models are almost identical. This is due the fact that the fluid temperature, in the one-field model, is assumed to be the same as the solid temperature and this assumption is thus satisfied (Bortolozzi & Deiber, 2000:167).

2.3.1.5 Implicit bed simulation models

This section discusses some of the simulation models that were developed by researchers. In these simulation models the presence of the spheres and pores were modelled implicitly through the use of the empirical correlations and models as discussed in the previous sections.

Jiang *et al.* (1999:1829) investigated the two-dimensional velocity distribution inside a rectangular packed bed by means of the discrete cell model. The concept of this model is to divide the bed into a number of interconnected discrete cells and allow the porosity to vary in two directions while it is assumed that the fluid flow is governed by the minimum rate of energy dissipation. Each cell can be assigned its own uniform porosity distribution. A major inability of this model is to account for the no-slip conditions at the wall interface. This problem is overcome by means of the ‘extra cell method’ through which an extra row of cells, with a very low porosity (i.e. less than 0.01), is added to account for the no-slip conditions at the wall interface (Jiang *et al.*, 1999:1831).

In order to obtain a high enough resolution of the bed properties and velocity distribution inside the bed, the cell size must be small compared to the bed scale. In order to apply the Ergun equation, each cell must however

be large compared to the particle scale. According to Holub (as cited by Jiang *et al.*, 1999:1831), three particle diameters can be considered appropriate for the discretization of the bed.

The rate of energy dissipation for each cell is formulated by means of the macroscopic mechanical energy balance (Jiang *et al.*, 1999:1842). The solution depends on the minimization of the rate of total energy dissipation for each cell (Jiang *et al.*, 1999:1832) with the mass balance being satisfied for each cell (Jiang *et al.*, 1999:1842).

The results obtained, from the discrete cell method, were verified by comparing them with the solutions obtained from the CFD code CDFLIB[®]. CDFLIB[®] is a solution algorithm which utilises a cell-centred finite-volume method in order to solve the time dependant conservation equations. In order to obtain consistency between the two methods, the discretization of the two model beds was the same (Jiang *et al.*, 1999:1833). Good agreement between the two methods was obtained, with the differences confined to within the 10% band (Jiang *et al.*, 1999:1829).

The discrete cell model can be utilised to predict the velocity distribution inside packed beds. The only problem is the discretization of the bed. With cell sized confined to a few particle diameters, the solution's resolution may not be high enough to be fully descriptive of the wall channelling phenomenon.

Another model used to study the performance of wall-cooled catalytic reactors is the lumped parameter model that assumes plug flow with a constant thermal dispersion coefficient (Cheng & Hsu, 1986:1843). In this model a derivative boundary condition with a finite wall heat transfer coefficient is assumed in order to account for the higher thermal resistance that is observed at the wall. This model is known to over predict the temperature hot spots in these reactors when the results obtained from the model are compared with experimental results. This may be attributed to the plug flow assumption, which does not account for the non-uniform radial velocity distribution (Cheng & Hsu, 1986:1843).

In the study conducted by Cheng and Hsu (1986:1843) they employed the Brinkman model with variable permeability as the momentum equation while an exponentially decaying correlation was used to describe the radial variation in porosity. From the porosity correlation and the viscous energy loss term from the Ergun equation they approximated the variation in permeability by an exponential function. In the model they assumed the fluid to be incompressible and that the inertial effect of the fluid is negligible (Cheng & Hsu, 1986:1845).

They obtained an analytical solution for the radial variation of the axial velocity by means of matched asymptotic expansion (Cheng & Hsu, 1986:1843). The inner cylinder diameter to particle diameter ratio's influence on the velocity distribution was also investigated. The dependency is shown in Figure 2-4 with γ

defined as d_p / R_t (Cheng & Hsu, 1986:1845). A decrease in particle diameter will thus result in a higher velocity peak being observed and that the peak moves closer towards the container wall.

In the model it is assumed that the inertial effect (i.e. velocity squared term in the momentum equation) of the fluid is negligible. This inertial effect must however be included when high speed forced convective flow through the bed is investigated. Due to the non-linear nature of this term a closed form analytical solution may not be obtained and numerical solutions may be considered in order to solve the velocity distribution (Cheng & Hsu., 1986:1851).

Bey and Eigenberger (1996:1365) investigated the velocity distribution through a cylindrical packed bed of spheres, rings and cylinders at different bed diameters. Their investigation included measurements made downstream of the bed and an axi-symmetric numerical simulation of the velocity distribution downstream of the packed bed. The basis of the model is the extended Brinkman equation and independently determined radial void fraction profiles. In the formulation of the model, the basic relations of the momentum balance were used (Bey & Eigenberger, 1996:1368). These relations were extended by means of the Ergun correlation in order to account for the pressure drop of the flow through the porous medium (Bey & Eigenberger 1996:1367). Rather than taking the inlet to the bed as the inlet to the computational domain, Bey and Eigenberger (1996:1969) took the inlet at a distance inside the bed where it could be assumed that the flow was fully developed, while the exit to the domain was taken as the exit of the empty tube, behind the packed bed. The bed in the experiment was supported on a monolith. The holes through the monolith had a width of 1mm and a length of 3.5mm with the fluid flowing downwards from the top of the bed into the monolith (Bey & Eigenberger, 1996:1366). The pressure drop due to the presence of the monolith was also included in the numerical simulation (Bey & Eigenberger, 1996:1369). In order to obtain a better fit between the measured and simulated results they replaced the laminar viscosity with an effective turbulent viscosity (Bey & Eigenberger, 1996:1368). The effective viscosity was determined by fitting the maximum simulated velocity to the measured velocity by means of a Gauss-Newton method (Bey & Eigenberger, 1996:1370).

The simulated results correlated well with the measured results after the introduction of the effective turbulent viscosity. The introduction of the effective viscosity implies that a measured velocity profile is needed in order to calculate the effective viscosity. If the bed type and set-up changes from the set-up used in this investigation, a new measured velocity profile is thus required in order to be able to predict the velocity distribution through the bed. The model gives no results on the development of the flow field inside the packed bed since the inlet to the computational field is situated a distance inside the bed where it can be assumed that the flow field is fully developed.

Ziolkowska and Ziolkowski (1993:3286) developed their mathematical model by dividing the bed into two separate regions i.e. the region near the wall (radius from wall ≤ 5 particle diameters) and the region in the

centre of the bed (radius from wall > 5 particle diameters). This has been done since the porosity in the near wall region oscillates up to a distance of approximately 5 particle diameters from the wall while the porosity in the centre of the bed approaches a constant value. The model was based upon the axial momentum equation while the resistance of the particles were modelled by means of the Ergun equation. The porosity variation was deduced from the experimental work of Benenati and Brislow (1962:360). The model also included an effective viscosity as one of the model parameters (Ziolkowska & Ziolkowski, 1993:3287). The effective viscosity was determined from measurements made downstream of the bed (Ziolkowska & Ziolkowski, 1993:3288). The calculated effective viscosity was found to be independent of the gas flow rate and the particle diameter while the profile resembled a damped oscillating function that approached zero (Ziolkowska & Ziolkowski, 1993:3289).

This model allows one to predict the radial distribution of the interstitial velocities for gas flow inside a cylindrical bed packed with spherical particles. All that is needed is the geometrical parameters of the bed along with the properties and average flow rate of the gas. The model does not require a measured velocity profile (Ziolkowska & Ziolkowski, 1993:3291).

If a different kind of bed (annular or rectangular) and particle geometry (deformed spheres or cylinders) is used the need may arise to recalculate the effective viscosity in order to predict the internal velocity distribution of the bed and this will necessitate a measured velocity profile. Another issue is that the model does not account for fluid flow downstream of the bed where velocity redistribution occurs. This is of interest in order to verify the predicted internal velocity distributions by means of a measured velocity profile made at the downstream of the bed.

Subagyo *et al.* (1997: 1375) developed a new mathematical model to predict the velocity distribution inside packed beds. In the development of the model the bed was divided into regions with voidage fractions higher than 0.5 and regions with voidage fractions lower than 0.5. By assuming that there is no fluid interaction between the voids in the regions of low voidage, the fluid flow for these regions is modelled after a set of tangled tubes constituting a discontinuous approach. The flow through the tubes is formulated by means of the Bernoulli equation (Subagyo *et al.* 1997:1377) while the Ergun equation is employed to account for the pressure drop. For the regions of high voidage this assumption does not hold true since fluid interaction between the voids do occur. For these regions the fluid flow was modelled after the flow around submerged objects by means of a continuous approach (Subagyo *et al.*, 1997:1376). The flow around these submerged objects is formulated by the viscous term of the axial momentum equation (Subagyo *et al.*, 1997:1378). This model also accounts for flow downstream of the bed and is formulated by the axial momentum equation (Subagyo *et al.*, 1997:1378). This is significant as velocity distributions measured downstream of a bed do not represent the velocity distribution inside the bed. This is due to the fact that flow redistribution starts as soon as the fluid exits the bed and the velocity profile start to approach the velocity distribution for flow through an

empty pipe (Subagyo *et al.*, 1997:1378). In the model the porosity distribution is calculated by means of the correlation proposed by Mueller (1992:272). Unlike some previous models, this model does not employ an effective viscosity as a correction factor to achieve a better fit between the measured and simulated velocity profiles. This improves the reliability of the model as no velocity measurements are needed in order to predict the velocity distribution inside the packed bed (Subagyo *et al.*, 1997:1383).

In terms of simplicity, only the fluid and bed properties need to be known in order to predict the velocity distribution inside the packed bed (Subagyo *et al.*, 1997:1380). This model can be applied to evaluate both compressible and incompressible fluid flows through a packed bed and compares well with previous models regarding accuracy (Subagyo *et al.*, 1997:1375).

All these models only describe the velocity distribution once it is assumed to be fully developed. None of these models describe the development of the profile in the inlet and outlet regions of the bed.

2.3.2 Explicit packed bed simulation models

As discussed previously, when the presence of the spheres and pores are modelled explicitly a number of key issues need to be addressed in order to obtain a high quality computational mesh. These issues include the treatment of the contact points between touching spheres along with the placement of a finer mesh on the surface of the spheres and around these contact points to prevent the generation of highly skewed cells in this region. Other issues to be addressed include the transition from a laminar to a turbulent flow regime and the use of a proper turbulence model. These issues will be discussed in the following section.

2.3.2.1 Contact handling

The treatment of the contact points is the most persistent issue regarding a computational mesh since the cells become highly skewed around the sharp angled geometry near the contact points (McLaughlin *et al.*, 2008) as shown in Figure 2-1.

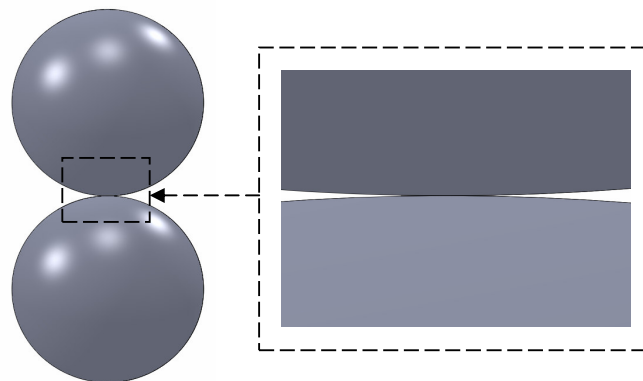


Figure 2-10: Sharp angle geometry at contact point (McLaughlin *et al.*, 2008)

During the generation of their computational mesh, Nijemeisland and Dixon (2001:236) modelled the contact points, between two touching objects, with common node on the surface of both touching objects. The fluid volume was then defined by placing two additional nodes on either surface. This procedure produced highly skewed (one surface of the tetrahedron is much larger than the others) fluid elements around the contact points. The skewed mesh did however not create any problems for their laminar solutions but convergence could not be achieved when the turbulent model was applied. It was discovered that flow velocities, particularly in the fluid elements around the contact points, increased dramatically.

In order to reduce the skewness of these fluid elements it was decided to create a gap between the entities (spheres and wall) in the geometry. The size of the gap was carefully determined since too small a gap would not eliminate the skewed elements and too large a gap would drastically influence the flow field in the system. The convective and conductive heat transfer mechanisms would also be affected since a considerable part of the conduction heat transfer in the bed occurs in the stagnant fluid around the contact points (Nijemeisland & Dixon, 2001:231). They found that the maximum sphere size, for which they could achieve a converged turbulent model, was 99.5%. Nijemeisland & Dixon (2001:237) also evaluated sphere sizes of 99, 97 and 95%. The velocity distributions obtained with 99% and 99.5% spheres showed good agreement with the velocity distribution obtained from the touching model when applied to laminar fluid flow. In their full study the 99% spheres model was used since it allowed for an easier model construction and faster convergence than the 99.5% sphere model.

A similar approach was followed by Logtenberg *et al.* (1999:2435) in the generation of their computational mesh.

Another approach followed in the literature is the replacement of the point contact with an area contact. Since the spheres will deform due to the gravitational loads on the bed this approach seems more reasonable than reducing the sphere diameter. The area based on contact treatment can be introduced into the model by either removing a cylinder of coolant from the fluid region or by reducing the pitch between the touching spheres.

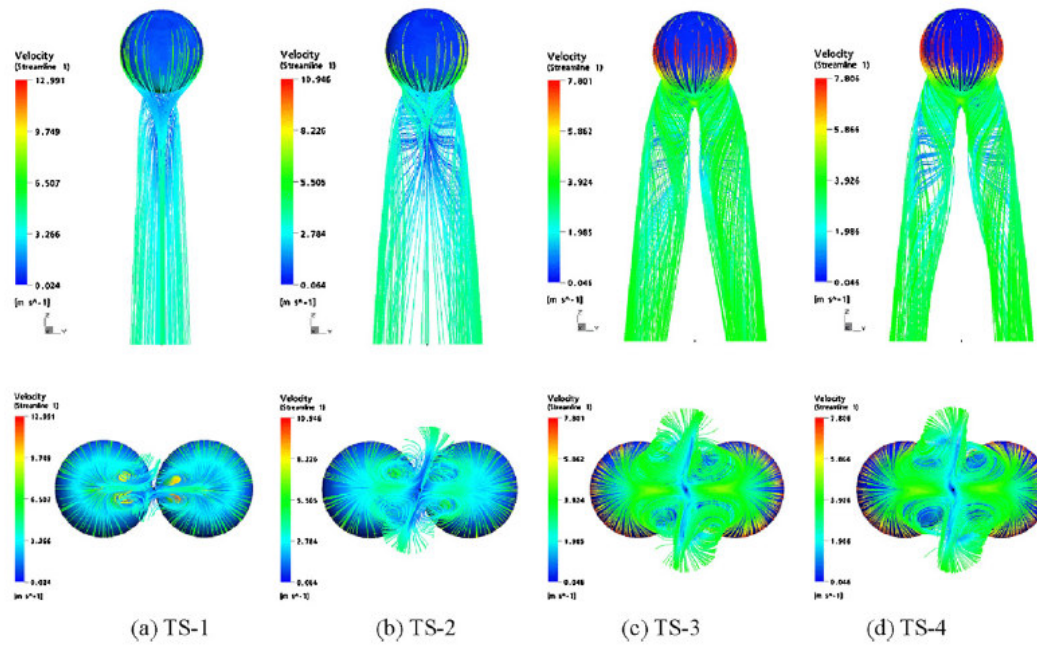
McLaughlin *et al.* (2008:3) followed the first approach by removing a cylinder of coolant from the fluid region where the diameter of the cylinder was determined from a Hertzian contact analysis. Wang-Kee In and Hassan (2008:2) employed direct area contacts by reducing the pitch between the spheres. No information about the pitch adjustments is however given.

Lee *et al.* (2007:2185) conducted an extensive study on the sensitivity of the numerical treatment of the contact points between spheres. In the investigation Lee *et al.* (2007:2185) used two horizontally aligned spheres with a diameter of 60mm. In each test case the pitch between the spheres was varied. A description of the different test cases conducted by Lee *et al.* is given in Table 2-2.

Table 2-2: Description of test cases conducted by Lee *et al.* (2007:2185)

TS-	Description	Sphere Dia. d_p (mm)	Pitch p (mm)	Contact Dia. d_{cont} (mm)	Number of nodes/elements
1	2 mm Gap	60	62	-	81,994/463,901
2	1 mm Gap	60	61	-	85,235/481,339
3	Point Contact	60	60	0	141,318/805,772
4	Area Contact	60	59.967	2	141,320/805,604

Lee *et al.* (2007:2187) found that the velocity profiles in the downstream region of the pebbles were greatly affected by the way in which the contact region was treated. Streamline profiles from test cases one and two compared favourably with one another while no significant differences were found between the point contact (test case 3) and the area contact (test case 4) studies. These results are shown in Figure 2-11.

**Figure 2-11: Streamlines downstream of spheres (Lee *et al.*, 2007:2187)**

From these results it is clear that special care should be taken in dealing with inter-pebble contacts as the flow distribution is greatly influenced by the contact treatment. Although the use of gaps, as an approximation for the contact regions between touching spheres, yields a computational mesh containing less nodes/elements and is thus less resource intensive, the physics of the fluids in the packing may be misinterpreted if there is an excessive approximation in the modelling of the inter-pebble contact region.

2.3.2.2 Mesh density

Mesh generation is probably the most important part in CFD modelling as it influences the accuracy of the model. A mesh must be fine enough to describe the flow field accurately but must also be coarse enough to

obtain a solution within a reasonable amount of time. Once a solution is deemed as grid independent further mesh refinements will increase both the model size and time needed to obtain a solution. Due to the complex geometry associated with packed beds most researchers have used unstructured grids with either uniform (Calis *et al.*, 2001; Tobis 2000) or scalable cell sizes (Wang-Kee In & Hassan, 2008; Lee *et al.*, 2007; McLaughlin *et al.*, 2008).

Calis *et al.* (2001:1716) used an unstructured mesh consisting of uniformly sized tetrahedral cells with an edge length of 1mm in their turbulent flow simulations while employing the $k-\varepsilon$ turbulence model. This corresponds to a particle diameter to cell-size ratio of $d_p / C_s = 12.7$. For their laminar flow simulations they combined a structured and unstructured mesh. The structured mesh consisted of five layers of prismatic cells and was generated adjacent to the sphere walls. From here an unstructured mesh, consisting of tetrahedral cells, was generated. In order to solve the boundary layer in the vicinity of the wall the thickness of the first prismatic cell was adjusted to 0.052 mm and then expanded at a rate of 1.2 over the remaining four prismatic layers while the tetrahedral cell size was taken as 0.4 mm. Tobis (2000:5364) also used an unstructured mesh consisting of equal sized tetrahedral cells of 2 mm with spheres of 38 mm ($d_p / C_s = 19$). In order to confirm mesh independence Tobis (2000:5365) reduced the cell size to 1 mm ($d_p / C_s = 38$).

Wang-Kee In and Hassan (2008:2) also used a combination of a structured and unstructured mesh similar to that of Calis *et al.* (2001). The added benefit was that the mesh had been locally refined and a higher mesh density could be observed near the contact points between the spheres. Their structured mesh consisted of 5 layers of prismatic cells. No information is however given on the cell sizes of the structured mesh. The unstructured mesh consisted of polyhedral cells with a minimum and target size of 0.3 mm ($d_p / C_{s-\min} = 200$) and 3 mm ($d_p / C_{s-\text{tar}} = 20$). McLaughlin *et al.* (2008:3) split their mesh around the contact points and these contact regions were meshed using quadrilateral cells. The rest of the pebble surface was meshed using tetrahedral cells. No information about the cell sizes is given but their final mesh consisted of approximately 160,000 cells per pebble.

The cell size/thickness adjacent to the pebble walls is of great importance for the application of wall functions. For turbulent flows the preferred range of the thickness of the near-wall cell layer is $30 \leq y^+ \leq 300$ (Calis *et al.*, 2001:1717). In the complex geometry of packed beds this criterion is difficult to satisfy since larger cell sizes can lead to highly skewed cells being generated in regions where spheres are in close proximity to each other. The alternative is to reduce the cell size in order to resolve the boundary layer ($y^+ \leq 1$) without the need for wall functions (Dixon *et al.*) This approach not only increases the model size but also increases the computational cost and time and is thus unsuited. Calis *et al.* (2001:1717) noted that the y^+ values varied by

factor of over 40 on the surface of the spheres. For the wall functions to be valid, the flow should also be fully developed which may not be the case for packed beds. All these factors will introduce a systematic error into the simulated pressure drop (Calis *et al.*, 2001:1717). Calis *et al.* (2001:1717) reported y^+ values of 4.4 at a Reynolds number of 100 and values of 440 at Reynolds numbers of 100,000. Guardo *et al.* (2005:1738) also noted y^+ values of $0.2 \leq y^+ \leq 20$. Despite applying wall functions outside their preferred ranges, Guardo *et al.* (2005:1739) still obtained good agreement between their simulated pressure drop and the theoretical pressure drop predicted by the Ergun equation.

2.3.2.3 Turbulence modelling

Knowledge of the laminar to turbulent flow transition range is crucial in order to correctly apply either laminar or turbulent flow models in the modelling of the packed bed.

Jolls and Hanratty (1966) found that the transition from laminar to turbulent flow occurred over a range of Reynolds numbers (based on the particle diameter and the fluid velocity in an empty tube) from 110 to 150. Similarly Logtenberg *et al.* (1999:2439) reported that no eddies were found inside the packing for Reynolds numbers smaller than 182. Hlushkou and Tallarek (2006:70) reviewed the analysis of flow regimes in porous media on both macroscopic and microscopic level. On a macroscopic level they concluded that there exist three flow regimes:

- creeping flow (linear laminar),
- viscous-inertial flow (non-linear laminar) and
- inertial flow (turbulent).

The transition from creeping flow to viscous-inertial flow occurs at Reynolds numbers ($Re_{inter} = \rho V_0 d_p / \mu_f \bar{\epsilon}$) of unity. The viscous-inertial flow regime lasts up to Re_{inter} of about 500 above which the turbulent flow regime dominates (Hlushkou & Tallarek, 2006:83).

On a microscopic level the transition from creeping flow to viscous-inertial flow occurs at a pore Reynolds number (based on the average pore size and average pore velocity) of about 30. Unsteady flow, indicating the end of the laminar flow regime, is observed at Reynolds numbers (as defined by equation (2.1)) of order 100 while microscopic turbulence begins at Reynolds numbers of order 300 (Hlushkou & Tallarek, 2006:83).

Thus for Reynolds numbers, as defined by equation (2.1), higher than 300 turbulence models should be applied. For the viscous-inertial region, $30 < Re < 300$, it is best to simulate the flow using both laminar and turbulent

flow models and compare the results afterwards in order to determine which approach yields better results. For Reynolds numbers smaller than 30 laminar flow can be assumed.

Due to the high computational demand of DNS, turbulence models are mostly used in simulations. These models have their own shortcomings and the application of the model to a situation, for which it was not derived, may adversely affect the simulation results. For this reason most CFD studies employ more than one turbulence model during the simulation process. These simulation models are then verified by comparing the predicted pressure drop to the theoretical pressure drop as predicted by the Ergun (1952) equation or similar pressure drop correlations. The selection of a proper turbulence model is thus essential for the proper simulation of the fluid flow phenomena present in packed beds.

McLaughlin *et al.* (2008:6) used the SST $k-\omega$, $k-\omega$ and RSM (Reynolds stress equation model) in their simulation of a randomly packed bed at Reynolds number of order 1×10^4 . McLaughlin *et al.* (2008:6) also succeeded in generating a mesh where the first prismatic layer yielded an y^+ value of less than 1. The KTA (1981) pressure drop correlation, equation (2.18), was used as verification for the simulated pressure drop. The simulated pressure drop, for all the turbulence models, showed excellent agreement with the theoretical pressure drop and fell within the error bounds of the pressure drop correlation. From their results McLaughlin *et al.* (2008:7) concluded that either of these turbulence models can be employed.

Wang-Kee In and Hassan (2008:3) used the Spalart-Allmaras, $k-\varepsilon$ and SST $k-\omega$ models with scalable wall treatment in their study of a staggered array of spheres at Reynolds numbers of order 6.5×10^4 . No information regarding the predicted pressure drop or y^+ values is given. It is only stated that the different turbulence models did not predict significant differences in the flow pattern around the spheres.

Calis *et al.* (2001:1717) employed the $k-\varepsilon$ and RSM turbulence models in their structured beds for a Reynolds number range of $1 \times 10^3 \leq Re \leq 1 \times 10^5$. In their study the y^+ criteria for wall functions was not met and y^+ values ranged from 4.4 at $Re = 1 \times 10^3$ to 440 at $Re = 1 \times 10^5$. They found that the RSM turbulence model yielded only slightly different pressure drop results (less than 10% discrepancy) from the $k-\varepsilon$ turbulence model. Calis *et al.* (2001:1717) considered this difference to be too small in order to justify the extra computational demand of the RSM model.

Guardo *et al.* (2005) investigated the influence of various turbulence models on the wall-to-fluid heat transfer in packed beds. In the evaluation they used the Spalart-Allmaras, Standard $k-\varepsilon$, RNG $k-\varepsilon$, Realizable $k-\varepsilon$ and Standard $k-\omega$ turbulence models. Their model consisted of 44 spheres and Reynolds numbers ranged from 1×10^2 to 1×10^3 . They were however incapable of producing a mesh which satisfied the y^+

criteria and their y^+ values were in the range of $0.2 < y^+ < 20$ making the mesh inadequate for the application of wall functions (Guardo *et al.* 2005:1738). Despite this fact, their CFD registered a pressure drop for each turbulence model, correlating well with the theoretical pressure drop proposed by the Ergun (1952) equation. They however noted that results from the Spalart-Allmaras turbulence model showed slightly better agreement with Ergun's (1952) predicted pressure drop.

It is thus clear that similar pressure drop results are obtained from all the above-mentioned turbulence models and that the more resource intensive models offer little improvement in accuracy over the simpler models. It can thus be concluded that the implementation of either of these turbulence models will yield acceptable pressure drop results.

2.4 Velocity measurement techniques

Although various advances have been made regarding velocity measurement instrumentation, it has so far been impossible to measure the velocity distribution inside a packed bed with a gas flowing through the bed (Bey & Eigenberger, 1996:1365).

These measurement techniques include the following:

- non-intrusive measurement techniques i.e.
 - Magnetic Resonance Imaging (MRI);
 - Nuclear Magnetic Resonance (NMR);
 - Laser Doppler Anemometry(LDA);
 - Particle Image Velocimetry (PIV);
- and intrusive measurement techniques i.e.
 - Hot Wire Anemometry
 - Pitot-Static tube.

2.4.1 Non-intrusive measurement techniques

Ogawa *et al.* (2001:174) made use of MRI to determine the pore structure and the internal three-dimensional velocity distribution in a packed bed. They considered a cylindrical bed with diameter 38 mm filled with crushed glass particles, sizes ranging from 2 to 5 mm, and spherical glass beads of 5mm diameter. In order to obtain results the use of the MRI technique requires that only the fluid flowing through the bed must be magnetically susceptible. In order to reduce the measurement time the fluid was doped with copper sulphate (Ogawa *et al.*, 2001:173). The flow velocity through the bed was very low, ranging from 3.84 to 13.2 mm/s (Ogawa *et al.*, 2001:172). For the bed, consisting of crushed glass, the corresponding Reynolds numbers were $Re = 10, 25$ and 40 (Ogawa *et al.*, 2001:177). For the bed, consisting of spherical particles, only one case with $Re = 19.3$ is discussed. Only a velocity map of the central vertical plane, showing the measured two-

dimensional velocity vectors is given (Ogawa *et al.*, 2001:179). No velocity distributions are shown. From the velocity map, regions near the wall with higher velocity vectors can be observed, indicating the presence of wall channelling (Ogawa *et al.*, 2001:179).

Lebon *et al.* (1996:296) made use of NMR to investigate the internal velocity distribution of a cylindrical bed packed with glass beads. The bed had an inside diameter of 8mm while the beads had a diameter of $800 \pm 150 \mu\text{m}$. The packing depth was 10 cm and the bed was retained by stainless steel grids with a $100 \mu\text{m}$ mesh sizes. In the study, flow rates of between 1.5 and 7.3 ml/min were used. These flow rates correspond to interstitial velocities of 1.3×10^{-3} and 6.7×10^{-3} m/s and Reynolds numbers of 0.36 and 1.8. No profile of the measured velocity distribution is given, only a graph representing the velocity probability distribution (Lebon *et al.*, 1996:298).

Giese *et al.* (1998:486) employed LDA to measure the velocity distribution inside a cylindrical bed packed with spheres, deformed spheres, cylinders and Raschig rings. The packing material (container, spheres, deformed spheres etc.) was manufactured from high quality Duran glass in order to minimize the scattering of the laser beam due to impurities. The cylinder had an inside diameter of 80 mm and was mounted on a high precision table which moved the bed in three directions, with an accuracy of ± 0.025 mm, via a computer. The liquid used in the investigation was a mixture of 95% dibutylphtalat and 5% ethyl alcohol. This mixture was used to match the refractive index of the glass (Giese *et al.*, 1998:484). In order to achieve a better signal, latex tracer particles were added to the fluid. The distance between adjacent velocity measurements was 1 mm, resulting in more than 5000 velocity measurements. From these interstitial velocities, the superficial velocities were obtained by averaging all the velocities at a fixed radius over the circumference, including the zero velocities measured inside the particles. They also measured the porosity distribution. The obtained porosity distribution resembles that of a damped oscillating profile (Giese *et al.*, 1998:485). The sphere diameter used in the investigation was 8.6 mm. For the bed consisting of spherical particles, the bed was exposed to various flow rates resulting in Reynolds numbers ranging from $\text{Re} = 4$ to 532. The obtained velocity profiles clearly indicate the presence of wall channelling and also the same damped oscillatory trend in accordance with the porosity distribution (Giese *et al.*, 1998:487). It is interesting to note that in the case of $\text{Re} = 4$, the second velocity peak exceeds the velocity peak at the wall. This may be due to the dependency of the velocity distribution on the Reynolds number at low Reynolds numbers and the resulting thickness of the wall boundary layer. What is also interesting to note is that the velocity peak observed decreases with an increase in Re . From the results the maximum measured superficial velocity is approximately 3.75 times more than the average superficial velocity through the empty cylinder.

Particle image velocimetry was used by Tchikango *et al.* (2006:2) to measure the velocity field of steady, laminar flow in the void spaces of a packed bed. The test section consisted of a 500 mm tube while spheres of diameter 9 mm and 30 mm were used as packing material. In order to achieve refractive index matching, all the

solid parts of the test section were fabricated from quartz glass while medical white oil (Shell Odina 927) was used as the fluid flowing through the packing. In order for the camera to detect the flow, fluorescent tracer particles were added to the fluid (Tchikango *et al.*, 2006:2). The flow through the bed was limited to 0.2 l/s corresponding to Reynolds numbers of $Re = 15$ and 45 . The three-dimensional velocity field was constructed from two-dimensional measurements made along various planes perpendicular to the mean flow field and plane parallel to the mean flow field. The latter measurements were made by rotating the bed to different positions in 10° increments. By using this technique, they were able to determine the axial velocity component from the three-dimensional flow field. By averaging the velocity in the mean flow direction and in the circumference, the radial distribution of the axial velocity was determined (Tchikango *et al.*, 2006:6). The obtained mean axial velocity distribution clearly illustrates wall-channelling occurring with the profile exhibiting the same form as a damped oscillating function. The influence of the tube to particle diameter ratio is also clearly evident as a higher velocity is observed in the packing with the smaller spheres.

The constraints involved with the use of MRI and NMR measurements techniques are that it is limited to non-magnetic and non-metallic materials (Tchikango *et al.*, 2006:1). Furthermore the cost involved in acquiring this instrumentation requires large financial investments. LDA and PIV requires transparent test sections and careful refractive index matching between the bed and the fluid being used in order to measure the interstitial velocities inside the bed. Since LDA uses constructive and destructive interference to detect the velocities, it is much more sensitive to variations in refractive indexes. With the use of PIV it is possible to obtain the velocity distribution in a plane while LDA is limited to point measurements, making the measurement times with LDA much longer than when using PIV (Tchikango *et al.*, 2006:1). PIV seeding is however needed in order for the camera to detect the particles movements. Of all the non-intrusive measurement techniques PIV is thus the most suited for measurements made inside the bed.

2.4.2 Intrusive measurement techniques

Schwartz and Smith (1953:1209) investigated the velocity distribution at the downstream of a cylindrical packed bed by using 5 circular hot wire anemometers at various radial positions. The cylinder diameters used in the investigation varied from 2 to 4 inches. They also investigated the effect of the distance between the exit of the bed and the plane of measurement on the measured velocity profile. If this distance is too large the velocity profile may be more descriptive of flow through an empty pipe rather than through the bed and if the distance is too small, velocity components perpendicular to the direction of flow may influence the measured velocity profiles. From their experimental investigation an optimal distance of 2 inches was found to be satisfactory (Schwartz & Smith, 1953:1212). The velocity profiles indicate that the maximum velocity is observed at a distance of one particle diameter from the wall (Schwartz & Smith, 1953:1214). For cylinder diameter to particle diameter ratios $D/d_p < 30$ the peak velocity ranged from 30% to 100% higher than the velocity observed in the centre of the bed. For cylinder diameter to particle diameter ratios $D/d_p > 30$ the peak velocity did not differ more than 20% from the velocity in the centre of the bed.

Price (1968:9) measured the velocity distribution at the downstream of a cylindrical packed bed with a 0.15 inch pitot-static tube in conjunction with a micro-manometer, with an accuracy of 0.001 inches of water. The cylinder had a diameter of 12 inches while the spheres had diameters of 0.25, 0.5 and 1 inches. A 5-mesh screen at the top and bottom of the bed contained the spheres. A honeycomb structure with a length of 4 inches was inserted between the plane of measurement and the top of the bed to ensure axial flow at the exit of the honeycomb. The design of the honeycombs consisted of annular rings joined together by radial vanes. Two honeycomb designs were used i.e. a constant area and a contracting area honeycomb. For the second design an area contraction ratio of 2.1 was found to be satisfactory and yielded good results which compared favourably with the first design. The obtained velocity distribution profiles clearly indicate the presence of wall channelling (Price, 1968:10). From the results it was deduced that the velocity distribution is independent of Reynolds number ($1470 < Re < 4350$) and bed length ($9 < L/d_p < 36$). A slight dependency on the tube diameter to particle diameter ratio was found ($12 < D/d_p < 48$).

Since the single sensor hot-wire anemometer cannot detect the direction of the flow, care should be taken not to take measurements too close to the exit of the bed as the turbulent flow will influence the measured velocity profile (Schwartz & Smith, 1953:1212). Another factor to consider is that in low velocity flows, natural convection, caused by the heating of the wire, will cause higher velocities to be measured. With the pitot-static tube, care should be taken that the micro-manometer or PDT (Pressure Differential Transmitter) should have an adequate range in order to detect the small pressure differences caused by very low velocities.

2.5 Conclusion

The velocity distribution through a packed bed strongly depends on the bed's geometrical parameters and fluid flow conditions. It was noted that the cylinder to particle diameter ratio (D_t / d_p) strongly affects the flow channelling inside the bed with more prominent velocity peaks observed closer to the beds containing walls with an increase in this ratio. The velocity distribution inside the packed bed is also dependant on the Reynolds number for $Re < 500$. For Reynolds numbers higher than 500, the dependency of the velocity profile on the Reynolds number no longer exists and the profile remains constant.

Two numerical modelling techniques have also been identified from the literature. In the first technique the presence of the spheres is modelled implicitly as a porous medium through the use of a porosity correlation that describes the packed bed's structure. The resistance of the pebbles is described by a pressure drop correlation along with an effective viscosity. This modelling technique only provides information on the average superficial velocity distribution inside the packing. No information is supplied on the intricate flow patterns around the spheres themselves. In the second modelling technique the presence of the spheres are modelled explicitly. With this technique the fluid flow around actual pebbles is solved for using commercial CFD RANS codes. This modelling approach however requires a large amount of computational resources and models are

normally limited to a small number of spheres. Due to resource limitations, the bed of the HTTU will be modelled using the implicit modelling technique (Chapter 5) while only a small section of the bed will be modelled explicitly (Chapter 4).

Various velocity measurement techniques have also been identified from the literature. A transparent packing and fluid (liquid) with identical refractive indices are required to be able to take measurements of velocity inside the packing using LDA and PIV. As the HTTU is not transparent and uses a gas, the velocity measurements can only be made downstream of the packing. Due to the high cost of PIV and LDA systems the use of a pitot-static tube or hot wire anemometer is thus preferred for this study. The use of a pitot-static tube is much simpler, but requires a pressure differential transmitter (PDT) capable of detecting very minute pressure differences. For this reason a hot wire anemometer is the most economical and adequate measurement technique for taking readings downstream of the bed.

The next chapter describes the experimental set-up and procedure used in the velocity tests.

Chapter 3

Experimental Set-up

3.1 Introduction

This chapter describes the experimental procedure that had been followed during the velocity measurements tests. The chapter starts of by describing the basic principles and components of a constant temperature anemometry (CTA) system. This is followed by an overview of the manner in which these instruments were set-up and the procedure followed during the velocity tests. The chapter concludes with a critical evaluation of the obtained velocity profiles.

3.2 CTA anemometer components and principles

The normal measuring equipment of a CTA system, constituting a measuring chain, is shown in Figure 3-1.

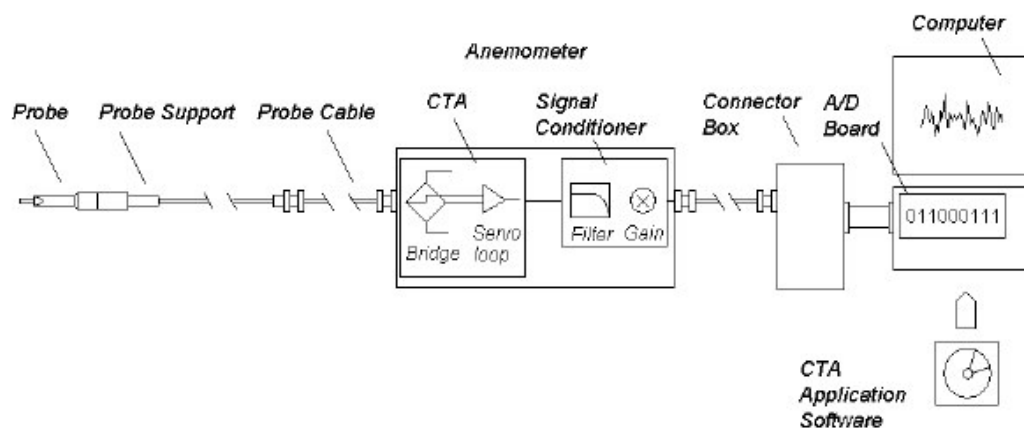


Figure 3-1: Typical CTA measuring chain (Jørgensen, 2002:6)

The anemometry measuring chain consists of five main components:

- probe with probe support and cabling,
- CTA anemometer,
- signal conditioner,
- A/D board & cabling and
- computer.

Normally dedicated application software forms part of the CTA anemometer that is used in the CTA system set-up, data acquisition and data analysis (Jørgensen, 2002: 6).

The CTA velocity measurements are based upon the heat transfer between the sensing element of the probe and the fluid flowing over the probe's sensing element. This is shown in Figure 3-2.

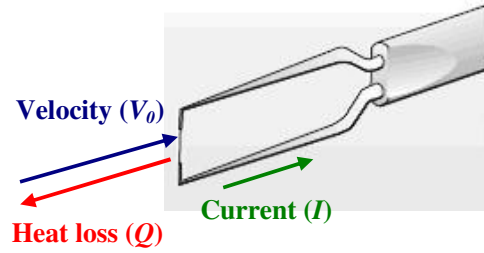


Figure 3-2: Heat loss from probe sensor

When a current (I) is passed through the probe's wire, heat is generated ($I^2 R_w$). During equilibrium, the heat generated in the wire is balanced by the convective heat loss from the wire to the surroundings (Jørgensen, 2002: 46). The relation between the heat generated and the convective heat loss from the probe's wire can be written as:

$$W = Q = I^2 R_w = hA(T_w - T_0) \quad (3.1)$$

where W constitutes the power generated by Joule heating, Q the heat transfer to surroundings, I the current passed through the wire, R_w the resistance of the wire, h the convection heat transfer coefficient, A the heat transfer area, T_w the temperature of the sensor and T_0 the temperature of the fluid at last overhear adjustment.

By replacing the convective heat transfer coefficient (h) with the Nusselt number (Nu) equation (3.1) can be rewritten as follow:

$$Q = I^2 R_w = \frac{A}{d_w} Nu k_f (T_w - T_0) \quad (3.2)$$

where d_w is the diameter of the wire and k_f is conductive heat transfer coefficient of the fluid.

The Nusselt number is calculated as:

$$Nu = A_1 + B_1 Re_w^n = A_2 + B_2 V^n \quad (3.3)$$

where Re_w is the wire based Reynolds number ($\rho V d_w / \mu_f$) and V the flow velocity past the wire and n, A_1, A_2, B_1 and B_2 constants.

Equation (3.2) can thus be written as (Jørgensen, 2002:47):

$$Q = I^2 R_w = (T_w - T_0)(A + BV^n) \quad (3.4)$$

A change in velocity will result in a change in the convective heat transfer coefficient. This will cause the wire temperature to change until a new equilibrium with the surroundings is obtained. Due to the thermal inertia of the wire it will not react instantaneously when exposed to changing velocities. This will result in a damped variation in wire resistance R_w causing flow fluctuations to be measured smaller than they actually are. In order to increase the response of the anemometer, compensation in the electronics of the anemometer is required. In a CTA system a feedback amplifier keeps the resistance and temperature of the wire constant. This procedure may increase the frequency limit of the anemometer by as much as a factor of 1000 (Jørgensen, 2002:46). Compensation in the anemometer electric circuit is provided by means of a Wheatstone bridge as shown graphically in Figure 3-3.

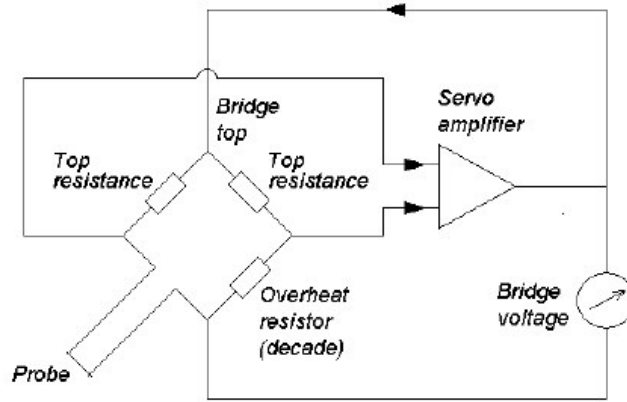


Figure 3-3: CTA anemometer principle diagram (Jørgensen, 2002: 51)

The hot-wire probe is placed in one arm of the Wheatstone bridge opposite a variable resistance resistor. This resistor defines the operating resistance and the operating temperature of the hot-wire. When the bridge is in balance, no voltage difference exists across its diagonal. When the velocity increases, the wire temperature and resistance will tend to decrease and an error voltage will exist at the input of the current regulating amplifier (Jørgensen, 2002:51). This error will cause the probe current to increase, which will heat and increase the resistance of the wire until the balance is restored (Jørgensen, 2002:51). The high gain of the current regulating amplifier causes the bridge to be in balance regardless of the flow velocity past the wire. The bridge voltage thus represents the probe current. Since all the resistances in the bridge are constant, the heat loss (Q) from the wire is directly represented by the squared bridge voltage (E^2) and can be replaced in the heat transfer equation (Jørgensen, 2002:51). The relation between the bridge voltage and the flow velocity past the wire can thus be written as:

$$V = \begin{cases} \left(\frac{E^2}{B} - \frac{A(T_w - T_0)}{B} \right)^{\frac{1}{n}} \\ C_0 + C_1 E + C_2 E^2 + C_3 E^3 + C_4 E^4 \end{cases} \quad \text{or} \quad (3.5)$$

where E is the CTA bridge voltage and A , B , C_0 , C_1 , C_2 , C_3 and C_4 are constants determined through the calibration of the anemometer.

Since the measurement principle of the CTA is based on heat transfer from the wire, measurements in non-isothermal flows will induce an error in the readings. Improper treatment of non-isothermal flows will result in an error in measured velocity of approximately 2% per 1°C change in fluid temperature (Jørgensen, 2002:37). The measured velocity will decrease with an increase in temperature and visa versa. For this reason it is important to adjust the measured bridge voltage before linearization and reduction. It is important to acquire both the ambient temperature (T_a) and the raw bridge voltage (E_a) to be able to account for temperature variations. The output voltage of the CTA bridge can thus be adjusted as follow:

$$E_{corr} = \left(\frac{T_w - T_0}{T_w - T_a} \right)^{0.5} \cdot E_a \quad (3.6)$$

where E_{corr} constitutes the corrected bridge voltage, T_w the sensor hot temperature, T_0 the reference fluid temperature during the last overheat adjustment before calibration and T_a the fluid temperature during acquisition

3.3 Test instrumentation

The Forced Convective Isothermal Tests (FCIT) were conducted in order to verify the velocity distribution models used in the design of the Pebble Bed Modular Reactor (PBMR) (Viljoen, 2008). The tests were conducted on the High Temperature Test Unit (HTTU) of the PBMR[®] which was designed and operated by M-Tech Industrial[®]. All the measurement instrumentation was sourced and designed by M-Tech Industrial[®]. The test design consisted of three major components i.e. the packed bed, the anemometry system and the traversing system for moving the probes above the bed.

3.3.1 Packed bed

Like the PBMR, the HTTU's bed consisted of an annular bed, packed randomly with 60 mm graphite spheres. The annulus had an inner radius (R_i) of 0.3 m and a height (L) of 1.2 m. The outer reflector wall of the annulus was not a cylinder. It consisted of 24 graphite straight segments that had been pieced together as illustrated in Figure 3-4.

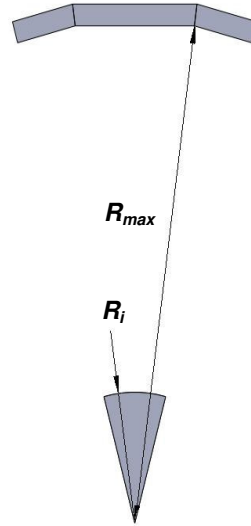


Figure 3-4: Illustration of inner and outer annulus walls

The maximum radius ($R_{\max}$) of the outer annulus wall was 1.15 m as shown in Figure 3-4. This caused the annulus to have an effective outer radius of 1.143 m. Due to the complexity of the outer annulus wall the wall was not perfectly circular but had a slight oval shape. Nitrogen entered the bed from the bottom and flowed vertically upwards.

3.3.2 Anemometry system

The anemometry system was purchased from Dantec Dynamics®. The components included the following:

- multi channel CTA system with mini CTA software and cables,
- two single sensor fibre-film probes (55R01),
- two 4mm dia. probe supports (55H21),
- reference velocity transducer (54T29), and
- reference temperature sensor (55P32).

The multi channel CTA system allows for multiple probes to be used simultaneously while the probe supports are used to connect the probes to the CTA system and allow the probes to be mounted at a point where velocity measurements are required. The velocity transducer provides a reference velocity measurement during the calibration of the probes. The reference temperature sensor is used to register temperature variations that occur during calibration and velocity acquisition. The temperature readings are also used during the temperature correction of the velocity measurements.

As mentioned previously, these tests were conducted in order to verify the axial velocity distribution models used in the design of the PBMR. The flow field above the bed is however very complex, non-steady and three-dimensional. The single sensor fibre-film probe only measures the velocity component perpendicular to the

wire. With the sensor of the probe orientated parallel to the z-axis, the probe will only measure the resultant (V_{xy}) of velocity components V_x and V_y when exposed to a velocity vector $\vec{V}$ as shown in Figure 3-5. The velocity readings were also direction independent meaning that the probe will not be able to distinguish between positive (flow exiting the bed) and negative (reverse flow into the bed) flow.

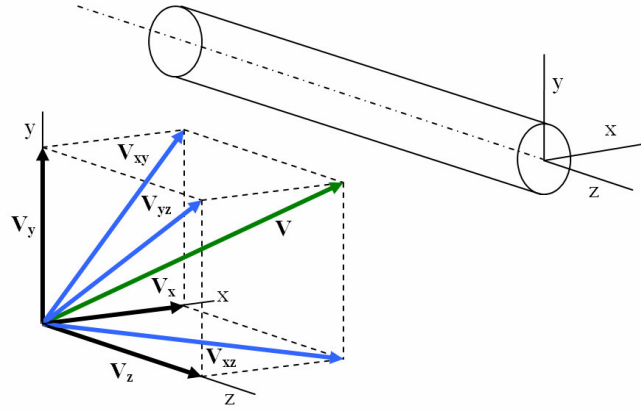


Figure 3-5: Velocity components measured by single sensor fibre-film probe

Other probes, like a triple-sensor probe, were considered but the fact that the probe's sensing wires weren't positioned at the same point meant that each sensor would effectively measure a different velocity. The set-up and calibration of these probes are more intricate and require additional calibration equipment, which would further increase the cost of the tests. For this reason it was decided that the current probes would yield sufficient information regarding the velocity distribution above the bed.

Another cause for concern is the fact that natural convection from the heated sensor wire would influence the velocity readings in very low flow rates. As the heat transfer from the heated sensor to the fluid moves from forced to natural convection a higher than actual velocity will be registered. This issue was addressed through the proper calibration of the wire in low fluid flow conditions.

The measured velocity profiles will thus contain an error if they are taken as the axial velocity distribution due to the inclusion of additional velocity component and direction independence of the probe readings.

3.3.3 Traversing system (TS)

The traversing system's primary function is to alter the position of the probes above the bed in order to take velocity readings downstream of the bed at different positions. The system and its control system were designed and built by M-Tech Industrial®.

The traversing system contains three different stepper motors to manoeuvre the probes through the flow field. The motion of the traversing system and probes, due to each individual motor, is shown schematically in Figure 3-6.

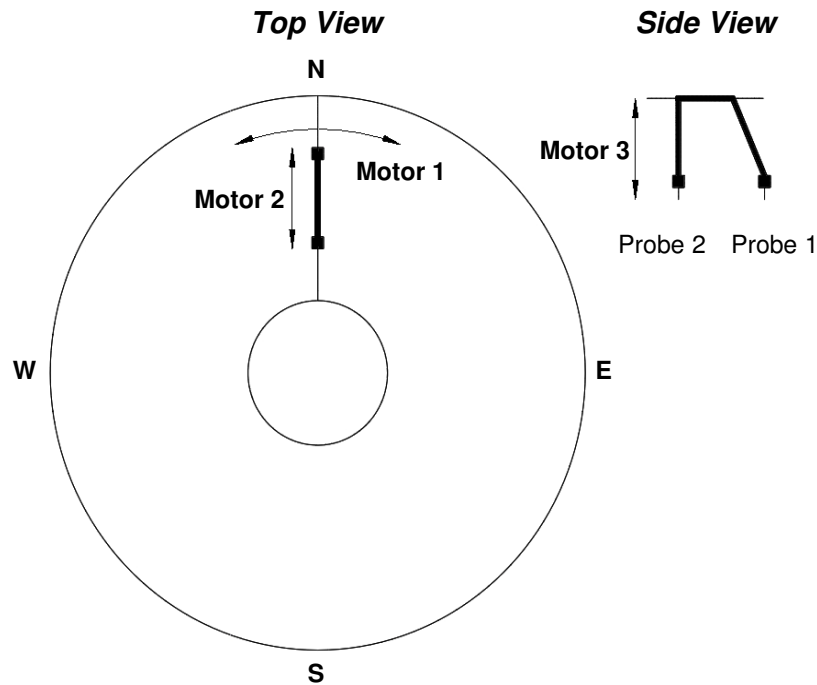


Figure 3-6: Traversing system's motion

As shown in Figure 3-6 two probes were used, with probe one positioned closest to the outer wall of the annulus (reflector) and probe two positioned closest to the inner annulus wall (heater). Since motor two only had a range of 0.48 m, the probes were mounted a distance of 0.37 m apart to be able to cover the entire radial span of the annulus (0.3 m to 1.15 m). The measuring region thus consisted of two independent regions. Velocity measurements would be carried out via probe one in the outer region of the annulus (0.725 m to 1.15 m) while probe two would be employed in the inner region of the annulus (0.3 m to 0.725 m).

Each motor has its own origin and zero point to which it will go to when given the command by the operator through the traversing system's graphical user interface (GUI) (Van Niekerk, 2008):

- Motor one rotates the probes as shown in Figure 3-6. The origin of motor one is at the North side of the bed, as shown in Figure 3-6 and this is designated as the zero degree point. When a measuring sequence is started the motor first moves the probes anti-clockwise to -15° . Once the probes are at -15° , the so-called "starting point" of motor one, the probes are rotated clockwise to 0° . From here the probes are rotated incrementally by a user defined angle increment. At a specified increment the probes are brought to a standstill. The probes are kept stationary for two seconds to allow the probe in use to acquire the velocity at the point of interest. From here the probes are moved to the next angle increment. This process is repeated until the probes have been rotated to 375° . Once this point is reached the probes are rotated anticlockwise to -15° to prevent a windup of the motor and probe wires.

While the probes are rotated anticlockwise, motor 2 moves the probes inward towards the centre of the annulus, to the next user specified radial position. This procedure is repeated until all the user specified radial increments have been completed.

- Motor two moves the probes inwards and outwards as shown in Figure 3-6. Motor two's origin is at the side of the annulus reflector and is controlled by a proximity switch. When the motor is given the 'origin' command, it will move the probes outward until it reaches the proximity switch where the motor's position will be reset. The origin and zero point differ for motor two. The zero point of motor two is between 1 and 20 000 steps (6 000 steps = 1 mm) inwards from the origin and can be set so that probe one is positioned exactly above the side of the reflector ($R_o = 1.15 \text{ m}$). As stated previously, the span of motor two is 0.48 m and probes one and two are mounted 0.37 m apart. Once motor two has moved 0.48 m inwards from its zero point probe two will be positioned above the side of the inner annulus wall (heater at $R_i = 0.3 \text{ m}$). In the case that the control system fails to stop motor two an emergency proximity switch was positioned a few millimetres inward from this endpoint to stop motor two. The whole radial span of the annulus is thus covered.
- Motor three moves the probes upwards and downwards as shown in Figure 3-6. Its origin is at the bottom slightly above the pebbles and is once again controlled by a proximity switch. Like motor two, motor three's zero point is not the same as the origin and is between 1 and 20 000 steps above the origin. The span of motor three is 75 mm upward from its zero point and can be adjusted to be a specified distance above the pebbles. An emergency proximity switch is located above the highest endpoint to stop the motor in case the control system is unable to do so.

A detailed explanation of the traversing system's GUI and the purpose of each button is provided in the document that can be found on the first disk included.

3.4 Instrumentation set-up

Prior to the execution of the velocity tests, the regions of interest in the flow field had to be identified. Secondly, the MiniCTA system had to be set-up and the probes calibrated.

3.4.1 Measurement Positions

Goodling *et al.* (1983:23) found that for cylindrical packed beds, the oscillation in porosity can be detected as far as five sphere diameters away from the cylinder wall. Since the velocity distribution is strongly effected by the porosity distribution, the greatest variation in velocity can be expected in these regions of oscillating porosity near the annulus walls. For this reason the measurement region above the bed was divided into three smaller regions. Regions one and three were situated closest to the annulus walls. The bounds of these two regions were situated a distance of five sphere diameters away from the walls. Region two was situated in the centre of the annulus. The three regions are shown in Figure 3-7.

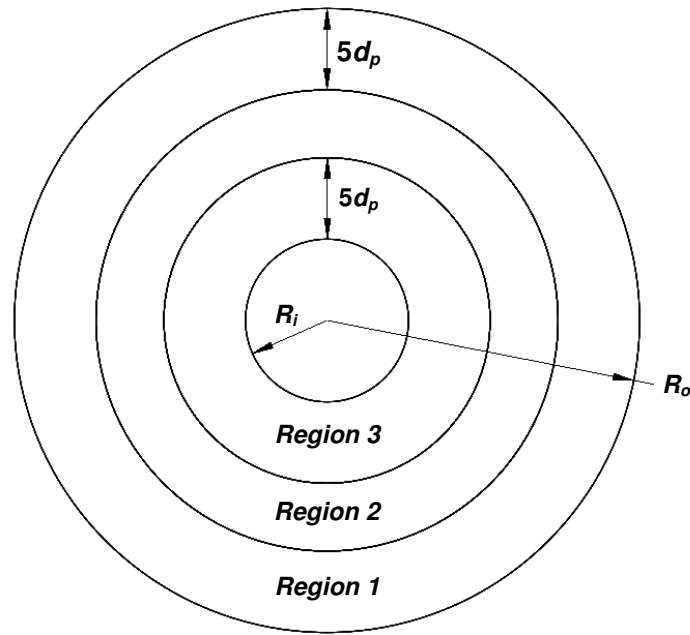


Figure 3-7: Fluid flow regions of interest downstream of the bed

To obtain a good indication of the oscillatory nature of the velocity distribution and wall-channelling phenomenon, measurements in regions one and three were made in radial increments of 15 mm ($d_p / 4$). Due to the relative constant porosity in region two the velocity was expected to be constant as well. For this reason the velocity was only measured at five radial positions. The span between these radial measurement positions, for region two, was thus 41.67 mm. Measurements in the circumference were made at angle increments of 3° , 4° and 6° for region one, two and three. These angle increments corresponded to an arc length of roughly 60 mm between successive measurement positions across the circumference. All the measurement positions can be seen in Figure 3-8.

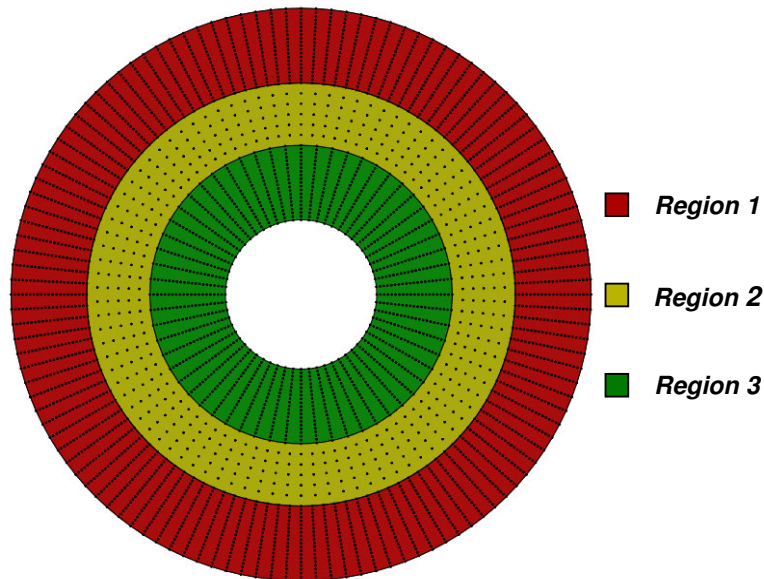


Figure 3-8: Velocity measurement positions

At each of the measurement positions, shown in Figure 3-8, 60 velocity readings were taken. These 60 velocity readings were averaged to obtain an average velocity for the point of interest. The average radial velocity was obtained by averaging all of the average point velocities at a specified radius. The average radial velocity is thus based on 7200, 5400 and 3600 velocity readings for regions one, two and three.

The zero-point of motor 2 was adjusted so that probe 1 is positioned at an outer annulus radius of $R_o = 1.15$ m. To prevent the probes from being driven into the pebbles when motor 3 is given the “Motor 3 to Origin” command, its lower proximity switch was moved upwards, away from the spheres. Defining the measurement height above the bed proved to be difficult as the height of spheres in the top level of the bed varied across the annulus and identifying the highest sphere in the packing is almost impossible. For this reason, motor 3 was moved to a distance of 60 mm upwards from its zero point. At this height 10 random readings of the distance between the probe’s sensing wire and the top of the pebble of interest were made. The average, maximum and minimum measured distances were 70.6 mm, 79.9 mm and 58.8 mm. For this reason motor 3 was moved upwards to a distance of 50 mm away from its zero point to be able to take velocity readings at an average height of about 60 mm from the bed.

When the probes were installed on the traversing system, they were orientated in such a way so that their sensing wires were tangential to the annulus. The probes would thus only measure the resultant of the axial and radial velocity components as discussed in section 3.3.2.

3.4.2 *MiniCTA probe calibration*

A custom calibration rig was built in order to calibrate the probes prior to their use in the velocity tests. Since the probe’s sensing wire is heated, natural convection will start to dominate the heat transfer from the wire rather than forced convection in low fluid flow conditions. This will cause the anemometry system to register a higher velocity than the actual velocity. To minimise the influence natural convection had on the velocity readings it was important that the probe’s orientation must be the same during calibration and the execution of the velocity tests. Secondly, since the fluid properties affect the heat transfer, it was deemed necessary that the same fluid, as was used during the velocity tests, be used during the calibration of the probes.

A representation of the calibration system and the manner in which the probes and other calibration equipment were installed are shown in Figure 3-9.

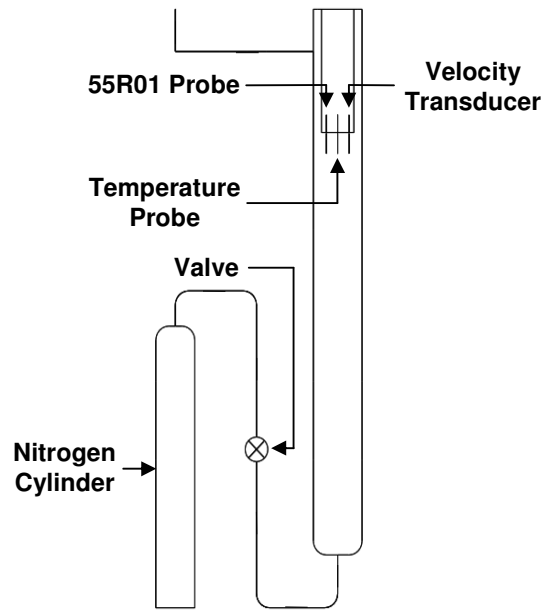


Figure 3-9: Calibration rig layout

For the calibration, nitrogen at a pressure of 200 bar, was fed into the system from a gas cylinder as shown in Figure 3-9. The gas leaving the system was fed into the atmosphere. The flow rate through the system was controlled by means of a gate valve. Because of the sudden pressure drop in the system (200 Bar to 0.875 Bar) the temperature of the calibration fluid did not remain constant. To monitor the change in gas temperature and to allow for temperature correction of the CTA bridge voltage, the reference temperature probe was also installed during the calibration. The reference calibration velocity was obtained through the use of the velocity transducer. The transducer contained a temperature-sensing probe and automatically corrected its readings for temperature variations.

All three probes were positioned in the centre of a 4-inch pipe with the gas flowing vertically over the probes. To ensure that the probe, being calibrated, and the velocity transducer were exposed to the same velocity, they were installed to be symmetrical around the centre of the pipe. The temperature probe was installed in the centre of the pipe. The probes were positioned a sufficient distance away from where the nitrogen was fed into the pipe to allow the velocity profile to be fully developed before the probes were reached.

A detailed description of the manner in which the anemometry system was set-up and the manner in which the calibration process was carried out, via the MiniCTA software package, is provided in the document on the first included disk. Both probes were calibrated using six reference velocity points. The generic form of the calibration curve, relating the corrected CTA bridge voltage to the velocity, is written as:

$$V(E_{corr}) = A \cdot E_{corr}^5 + B \cdot E_{corr}^4 + C \cdot E_{corr}^3 + D \cdot E_{corr}^2 + E \cdot E_{corr} + F \quad (3.7)$$

where the coefficients of equation (3.7) is give in Table 3-1.

Table 3-1: Probe calibration curve coefficients

<i>Coefficient</i>	<i>Calibration 1</i>		<i>Calibration 2</i>	
	<i>Probe 1</i>	<i>Probe 2</i>	<i>Probe 1</i>	<i>Probe 2</i>
A	3.17463	-3.21749	0.79093	2.66174
B	-30.82693	30.11631	-7.54522	-25.33057
C	119.26761	-110.24385	29.47366	95.80148
D	-228.92472	198.35745	-57.58243	-178.35573
E	218.74496	-174.59726	56.67406	163.90125
F	-83.45295	59.8883	-22.59963	-59.6068

To serve as a check of the quality of the calibration, the velocity in the centre of the annulus ($r = 0.725$ m) was measured using both probes. The average velocity at this radius was measured at 0.583 m/s using probe 1 and 0.572 m/s using probe 2. The difference between these readings was 0.011 m/s, which corresponded to a percentage difference of 1.89%. The difference was lower than the probe's uncertainty of 0.02 m/s (Stannov, 2007), which leads to confidence in the calibration of the probes.

A second calibration of the probes was carried out after the velocity tests were completed. This was done in order to quantify the amount of drift the probes experienced during the velocity tests due to fouling of the probe's sensing wire. The calculated drift of each probe was used in the uncertainty analysis of each probe and is discussed in the next section.

3.5 Test execution & Uncertainty analysis

This section provides an overview of the manner in which the velocity tests were carried out along with the manner in which the uncertainty, pertaining to the velocity measurements, was obtained.

3.5.1 Velocity test execution

The velocity tests were carried out under forced convective isothermal fluid flow conditions. The tests were conducted under mass flow rates of 0.5, 1.0, 2.0, 3.0 and 4.0 kg/s of pure nitrogen. This corresponded to pebble based Reynolds numbers of 438, 877, 1754, 2631 and 3508 for nitrogen at a temperature and pressure of 20° and 100 kPa. A test set, named Forced Convective Isothermal Test (FCIT), consisted of velocity measurements at each of the specified mass flow rates. In order to establish the repeatability of the velocity profiles, three test sets (FCIT1, FCIT2 and FCIT3) were conducted in succession. As mentioned, the tests were conducted under isothermal conditions while the system pressure was kept constant at 100 kPa.

The manner in which the Mini CTA system was set-up using both probes, their respective calibration data and the reference temperature probe are discussed in the document on the first included disk.

Since the velocity measurements of the MiniCTA system was exported in a *.CSV file, the number of readings which could be taken in one run was limited by the number of rows in an EXCEL[®] spreadsheet. For this reason a test, at a specified mass flow rate, was broken down into smaller segments. Each of these smaller segments consisted of velocity measurements across the circumference at a specified radius. The exported *.CSV file, from the anemometry system, contained the temperature corrected velocities of both probes, the temperature, as measured by the temperature probe, and the date and time at which each reading was made.

The traversing system was set-up to move the probes across the circumference, at a designated radius, and to bring the probes to a halt for two seconds at specified angle increments. All measurements were made at a height of 60 mm from the bed. At the end of the traversing sequence the relevant information was automatically exported to a *.CSV file. This file contained the radius at which the probes were traversed, the date, time and angle at which the probes were stationary, and the probe that had been used during the traversing sequence.

Van Niekerk (2008) developed an EXCEL[®] based spreadsheet which time-matched the velocity readings to the angles where the probes were stationary. This file contained all the information regarding the measuring sequence, i.e., the radius at which the traverse was made, the probe that was used to measure the velocity, the angle increments at which the probe was stationary, the average velocity at the specific angle increments and the standard deviation associated with the average velocity. The sampling rate of the anemometry system was set to 30 Hz. This meant that 60 readings were taken per angle increment where the probe is stationary. All these positions are shown in Figure 3-8. From these 60 velocity readings the average velocity for the point of interest was calculated as follows:

$$\overline{V_0(r, \theta)_p} = \frac{\sum_{i=1}^n V_o(r, \theta)_i}{n} \quad (3.8)$$

where n is the number of readings taken at the point where the probes were stationary, r and θ the radial and tangential positions where the readings were made, $V_o(r, \theta)_i$ is the i^{th} superficial velocity reading taken at the point (r, θ) and $\overline{V_0(r, \theta)_p}$ is the average superficial velocity of the point (r, θ) .

All these average point velocities at a specific radius were then averaged in order to obtain an average superficial velocity for the corresponding radius. This average velocity was calculated as follows:

$$\overline{V_0(r)} = \frac{\sum_{i=1}^n \overline{V_o(r, \theta)_i}}{n} \quad (3.9)$$

where n is the number of average point velocities found on the radius of interest, $\overline{V_0(r, \theta)_i}$ is the i^{th} average point velocity at the specific radius as calculated from equation (3.8) and $\overline{V_0(r)}$ is the average velocity corresponding to the radius r .

The experimental procedure used to obtain these average velocities, at a specific radius, is discussed in greater detail in the document on the first included disk.

This process was repeated for each of the radial positions at which the velocity had to be obtained. These average superficial velocities $\left(\overline{V_0(r)}\right)$ were then used to generate the average radial velocity distribution. Once a test at a specific mass flow rate was concluded, then the whole procedure was repeated for the next mass flow rate. At higher mass flow rates the blowers, used to circulate the nitrogen, would cause the nitrogen to heat up. To ensure that the test were conducted under isothermal conditions, velocity measurements were put on hold until the bed and gas temperatures reached a steady state.

3.5.2 Uncertainty analysis

The uncertainty of a measurement serves to indicate the margin of error present in the measurement. The uncertainty of a data series has three contributing factors i.e. the uncertainty of the instrument used in the experiment, the standard deviation between the measurements in the data set and the drift the instrument experienced during the acquisition of the data set. The uncertainty of measurement can thus be formulated as follows (Stern *et al.*, 1999):

$$U_p = \sqrt{U_{stdev}^2 + U_{inst}^2 + U_{drift}^2} \quad (3.10)$$

where U_p is the uncertainty of a set of measurements, U_{stdev} is the standard deviation between measurements in the data set, U_{inst} the instrument uncertainty and U_{drift} the drift the instrument experienced.

Since the average point velocities were calculated from 60 velocity readings the sample standard deviation for these measurements can be calculated as follows:

$$U_{stdev} = \sqrt{\frac{n \sum_{i=1}^n V_i^2 - \left(\sum_{i=1}^n V_i \right)^2}{n(n-1)}} \quad (3.11)$$

where n is the number of readings in the data set ($n = 60$) and V_i the i^{th} velocity reading in the data set.

The instrument uncertainty (U_{inst}) was taken as $U_{inst} = 0.02$ m/s (Stannov, 2007). The drift (U_{drift}) an instrument experienced can be explained using Figure 3-10.

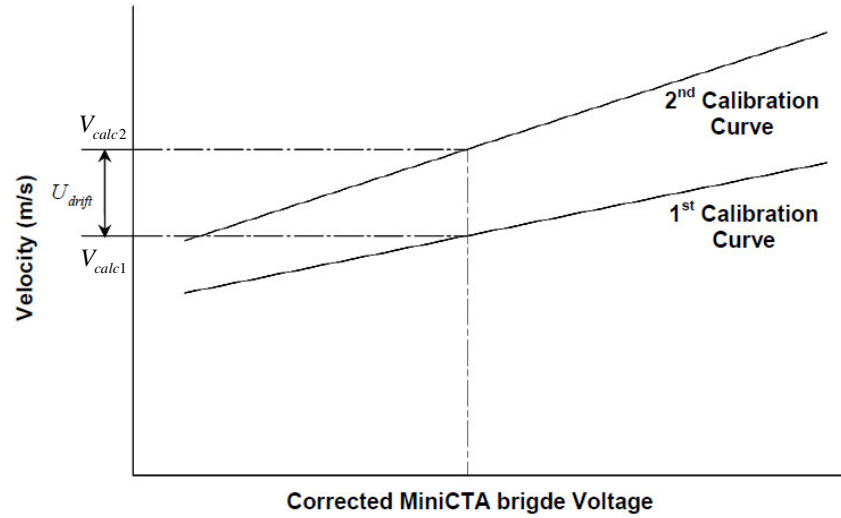


Figure 3-10: Instrument drift definition

For a certain corrected MiniCTA bridge voltage (E_{corr}) equation (3.7) with the coefficients of calibration 1, given in Table 3-1, yields a corresponding velocity (V_{cal1}). For the same bridge voltage the second calibration curve yields a different velocity (V_{cal2}). The difference between these two velocities equals the drift of the instrument at the particular voltage. Similarly the average drift of the probe, over the entire span of voltages, can be calculated as follow:

$$U_{drift} = \left| \frac{\int_{E_{corr_{min}}}^{E_{corr_{max}}} V_{cal1}(E_{corr}) dE_{corr} - \int_{E_{corr_{min}}}^{E_{corr_{max}}} V_{cal2}(E_{corr}) dE_{corr}}{E_{corr_{max}} - E_{corr_{min}}} \right| \quad (3.12)$$

where $E_{corr_{max}}$ and $E_{corr_{min}}$ are the maximum and minimum corrected MiniCTA bridge voltages encountered during the calibration of the probe; $V_{cal1}(E_{corr})$ the velocity from the first calibration curve and $V_{cal2}(E_{corr})$ the velocity from the second calibration curve.

For the uncertainty analysis of the HTTU the average drift approach was employed. For probe one the integrals were calculated for $E_{corr_{min}} = 1.4$ V and $E_{corr_{max}} = 2.3$ V. For probe two the minimum and maximum corrected voltages, used in the calculation were $E_{corr_{min}} = 1.3$ V and $E_{corr_{max}} = 2.18$ V. The average drift of probe one was calculated as 0.0246 m/s. For probe two the average drift was calculated as 0.0143 m/s.

Using these values the uncertainty for each of the average point velocities were calculated using equation (3.10)

The uncertainties of all the average point velocities $\left(\overline{V_o(r, \theta)_p}\right)$, at a specific radius, were then combined to obtain the uncertainty of the average velocity $\left(\overline{V_o(r)}\right)$ associated with the radius in question. This uncertainty was calculated as follows (Stern *et al.*, 1999):

$$U_{avg} = \sqrt{\frac{1}{n^2} \sum_{i=n}^n U_i^2} \quad (3.13)$$

where n is the number of average point velocities used to calculate the average velocity at the particular radius and U_i is the i^{th} uncertainty of the average point velocity as defined in equation (3.10).

3.6 Results & Discussion

The velocity profiles, for each of the three test cases, at mass flow rates of 0.5, 1.0, 2.0, 3.0 & 4.0 kg/s are shown in Figure 3-11 to Figure 3-15. The Reynolds number listed in the figures are the average Reynolds number of the three tests since the temperature of the nitrogen varied between each test. The error bars in the graphs represent the uncertainty of the velocity reading and were calculated as described in the previous section. A summary of the maximum uncertainty, as a percentage of the velocity, for each of the listed velocity profiles is provided in Table 3-2.

Table 3-2: Maximum uncertainty of velocity profiles

<i>Mass Flow (kg/s)</i>	<i>Maximum Uncertainty</i>		
	<i>FCIT1</i>	<i>FCIT2</i>	<i>FCIT3</i>
0.5	6.60%	6.53%	6.59%
1.0	5.18%	5.30%	5.24%
2.0	4.25%	4.41%	4.34%
3.0	4.11%	4.18%	4.04%
4.0	3.98%	3.99%	3.97%

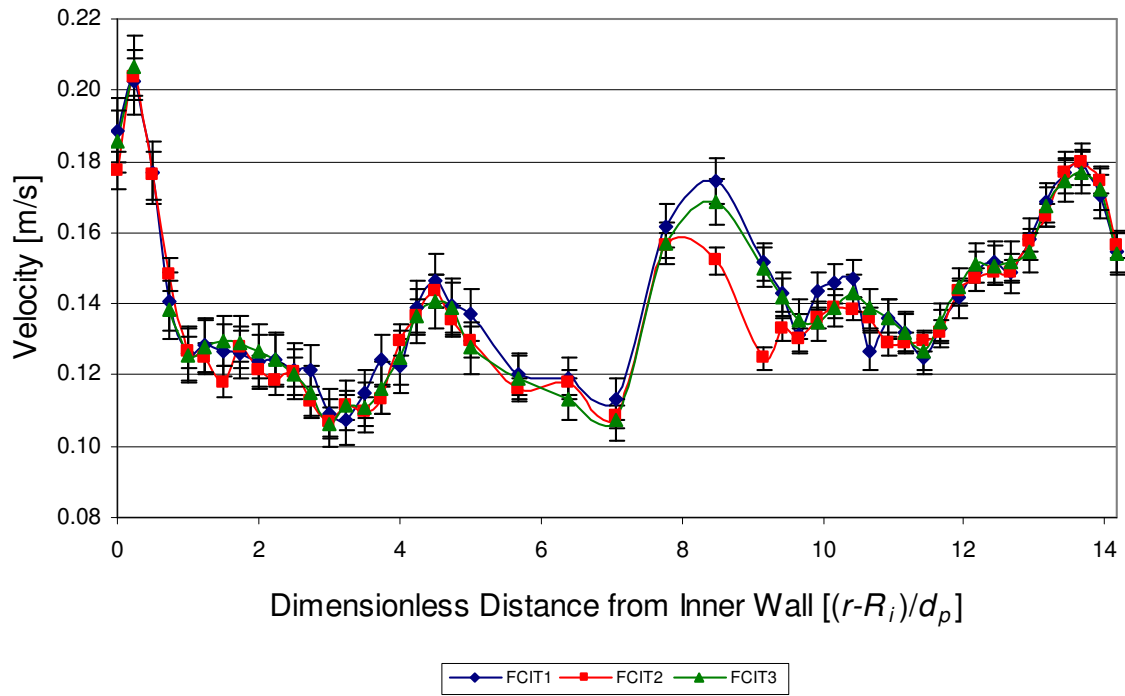


Figure 3-11: Velocity distribution at a mass flow of 0.5 kg/s (Re=439 & $V_0 = 0.114$ m/s)

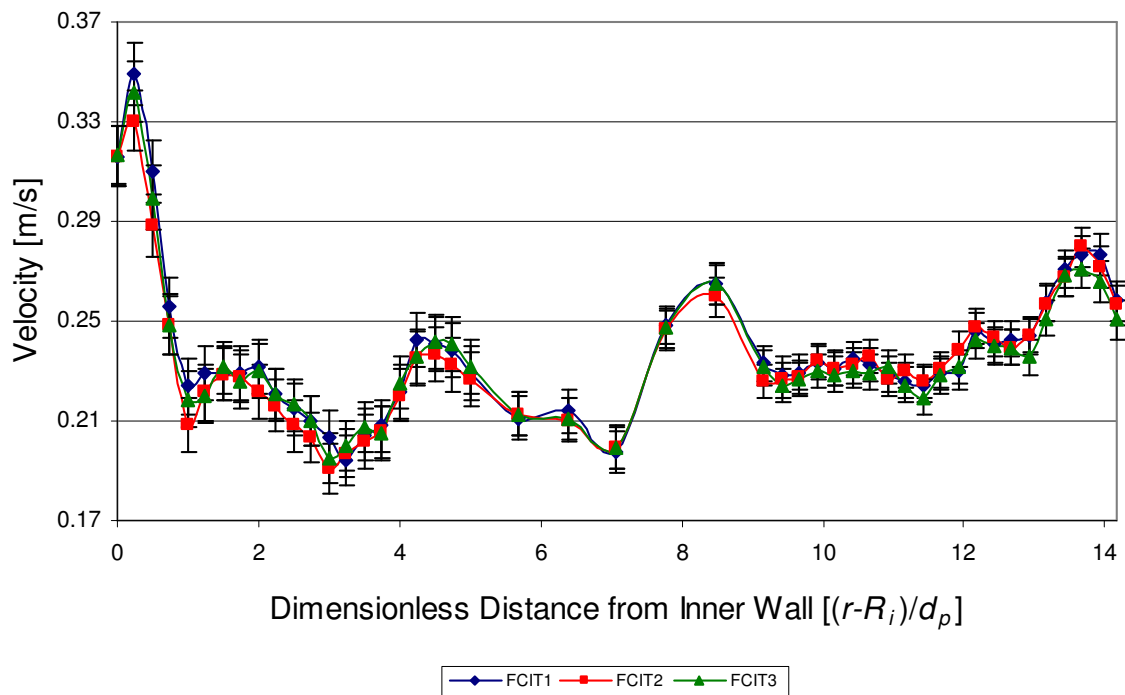


Figure 3-12: Velocity distribution at a mass flow of 1.0 kg/s (Re=883 & $V_0 = 0.226$ m/s)

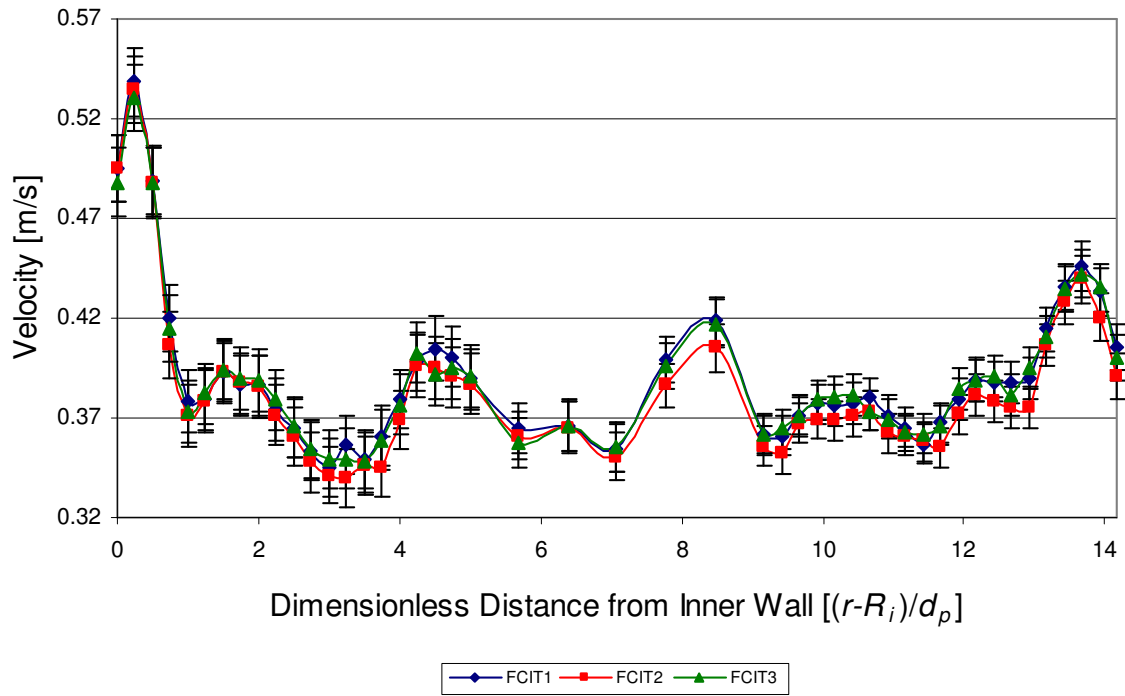


Figure 3-13: Velocity distribution at a mass flow of 2.0 kg/s ($Re=1753$ & $V_0 = 0.456$ m/s)

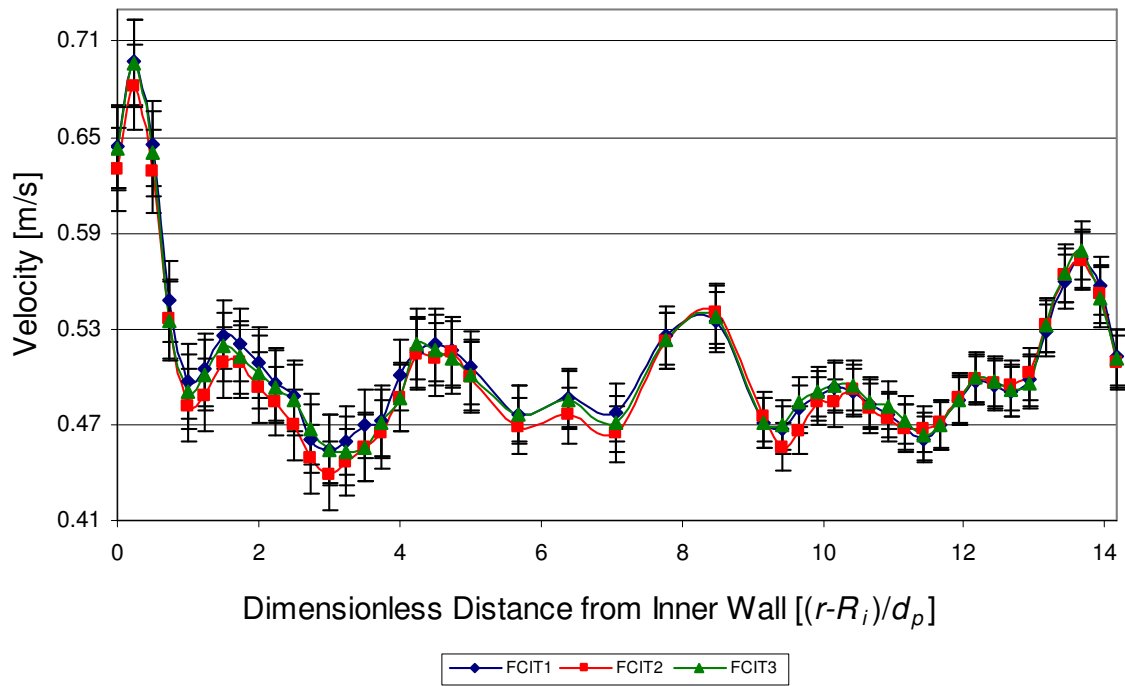


Figure 3-14: Velocity distribution at a mass flow of 3.0 kg/s ($Re=2626$ & $V_0 = 0.685$ m/s)

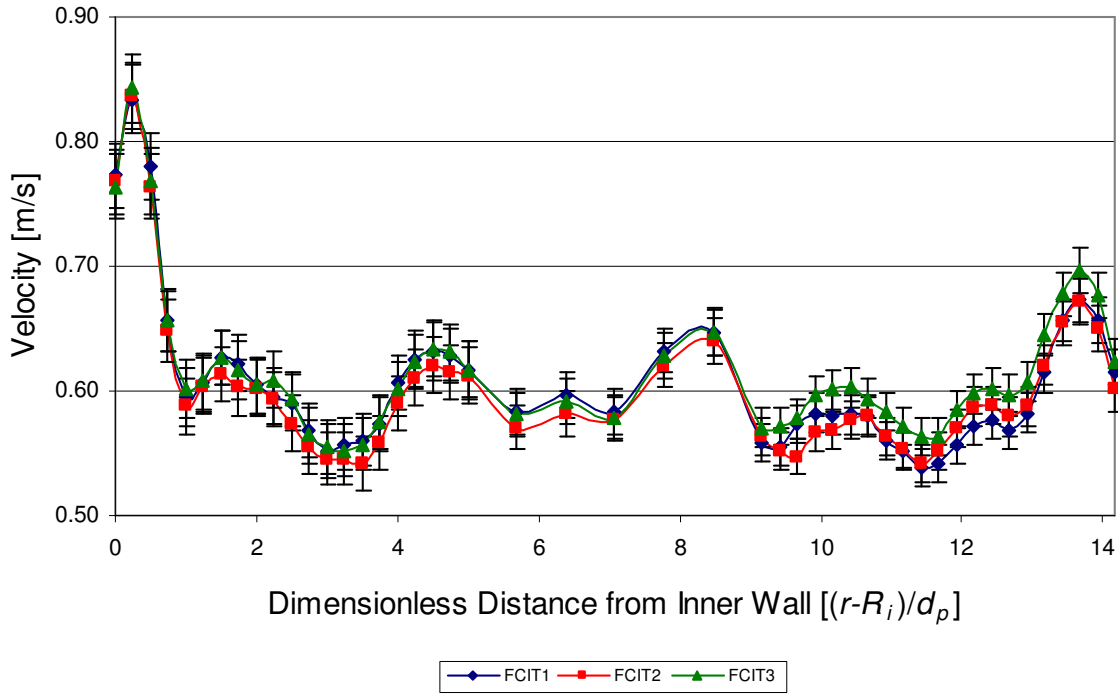


Figure 3-15: Velocity distribution at a mass flow of 4.0 kg/s ($Re=3453$ & $V_0 = 0.929$ m/s)

From the listed figures it can be seen that the velocity profiles, for each test, show good agreement with each other. The profiles fall within each other's uncertainty/error bands. This repeatability strengthens the confidence in the velocity measurements. All the velocity profiles, at the different mass flow rates, exhibit the same trend. In all the cases the peaks and dips in the velocity profile are observed at the same radial positions. In each of the velocity profiles a significant peak in the velocity profile can be observed near the inner annulus wall. This indicates the presence of wall channelling. The velocity peak near the outer annulus wall is however less pronounced. A clarification on the absence of the outer velocity peak will be given later in this section.

It is also noted that the measurements, obtained at lower mass flow rates, exhibit a larger uncertainty as shown in Table 3-2. This indicates that at a lower mass flow rate, the measurements contained more noise. This is supported by the turbulence intensities that had been calculated at the various mass flow rates. The average turbulence intensity for each of the velocity tests is given in Table 3-3.

Table 3-3: Average turbulence intensity at various mass flow rates

<i>Mass Flow (kg/s)</i>	<i>FCIT1</i>	<i>FCIT2</i>	<i>FCIT3</i>
0.5	61.42%	62.64%	61.59%
1.0	50.14%	50.35%	50.34%
2.0	44.10%	44.62%	44.12%
3.0	42.67%	43.02%	42.73%
4.0	42.40%	42.34%	41.90%

As seen from Table 3-3, higher turbulence intensities were observed at lower mass flow rates. Turbulence intensity is a measure of the amount and magnitude by which the velocity varies at a point in all directions. At low mass flow rates the measurements contained a greater variation in velocity (standard deviation), which would explain the higher uncertainty values. A possible explanation for the reduction in turbulence intensity with an increase in mass flow rate can be found by looking at the shedding vortices (Von Kármán Vortex Street) behind spheres and cylinders (Houghton & Carpenter, 1993:345). At Reynolds numbers ranging from $100 < Re < 400$ large vortices are shed from the cylinder periodically. With an increase in Reynolds number the periodic shedding of vortices stop and a wide turbulent wake, containing smaller random vortices, forms behind the sphere. These larger vortices, at lower mass flow rates, may cause a large variation in the velocity readings. This in turn will result in higher turbulence intensities, as was the case in the velocity tests at lower mass flow rates.

Direct comparison of the profiles, through normalization by means of the empty annulus superficial velocity (V_0), was not possible. As mentioned previously, the measured velocity profiles represent the resultant of the axial and radial velocity components. For this reason the velocity profiles were normalised using the mass flow rate that was calculated by integrating the velocity profiles over the entire area of the annulus. This integration yielded a volume flow rate. Using the average temperature and a pressure of 100 kPa, the properties of the gas for each test were determined. The average temperature was monitored using the CTA system's reference temperature probe. Using these gas properties, the mass flow rate was determined and the associated empty annulus superficial velocity (V_{0calc}).

At low mass flow rates the calculated mass flow rate was higher than the mass flow rate used during the velocity tests. This was expected since the measured velocity profile did not represent the distribution of the axial velocity component. It included the radial velocity component. At higher mass flow rates the calculated mass flow rate was lower than the mass flow rate that was used during the velocity tests. The percentage deviation between the calculated and actual mass flow rate, for each test, is shown in Figure 3-16.

An over prediction of the mass flow rate was expected due to the inability of the probes to solely measure the axial velocity component and to distinguish between positive and negative fluid flow. Like the reduction in turbulence it could be argued that the percentage deviation between the calculated and actual mass flow rates would systematically become smaller with an increase in mass flow rate.

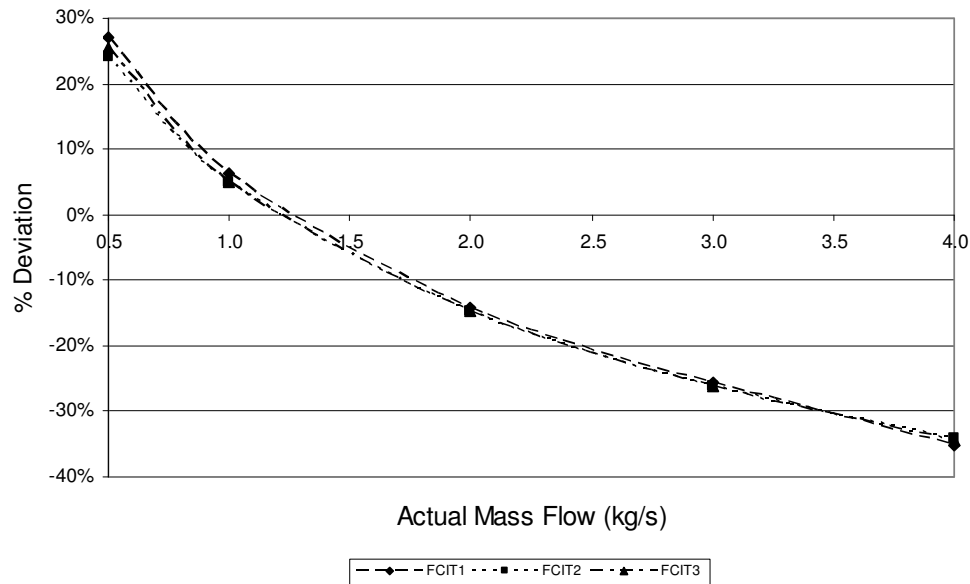


Figure 3-16: Percentage deviation between calculated and actual mass flow rate

As described previously, at higher mass flow rates, the vortices become smaller and more random. This implies that even though the radial velocity component may stay the same, the increase in the axial velocity component would reduce the influence the radial velocity component has on the measured velocity. The measured velocity would thus approach the axial velocity component with an increase in mass flow rate and the calculated mass flow rate would thus approach the actual mass flow rate.

The fact that the calculated mass flow rates are lower than the actual mass flow rates point to either a problem with the probes or a measuring technique error. The problem most likely lies with the velocity transducer used to calibrate the probes. This could however not be verified as the velocity transducer was never sent away for recalibration after the velocity tests were concluded since the high shipping and recalibration costs wasn't justified.

The error seems to be systematic across the entire measurement range. The influence of this error could be minimized if the velocity profiles were normalised using the calculated superficial velocity (V_{0calc}) calculated from the calculated mass flow rate. Since the normalizing velocity contained the same error as the velocity profile, the measurement error will be minimized. The normalized velocity profiles are shown in Figure 3-17. These profiles represent the average velocity profile that was calculated from the three repeatability test profiles (FCIT1, FCIT2 & FCIT3) for each mass flow rate.

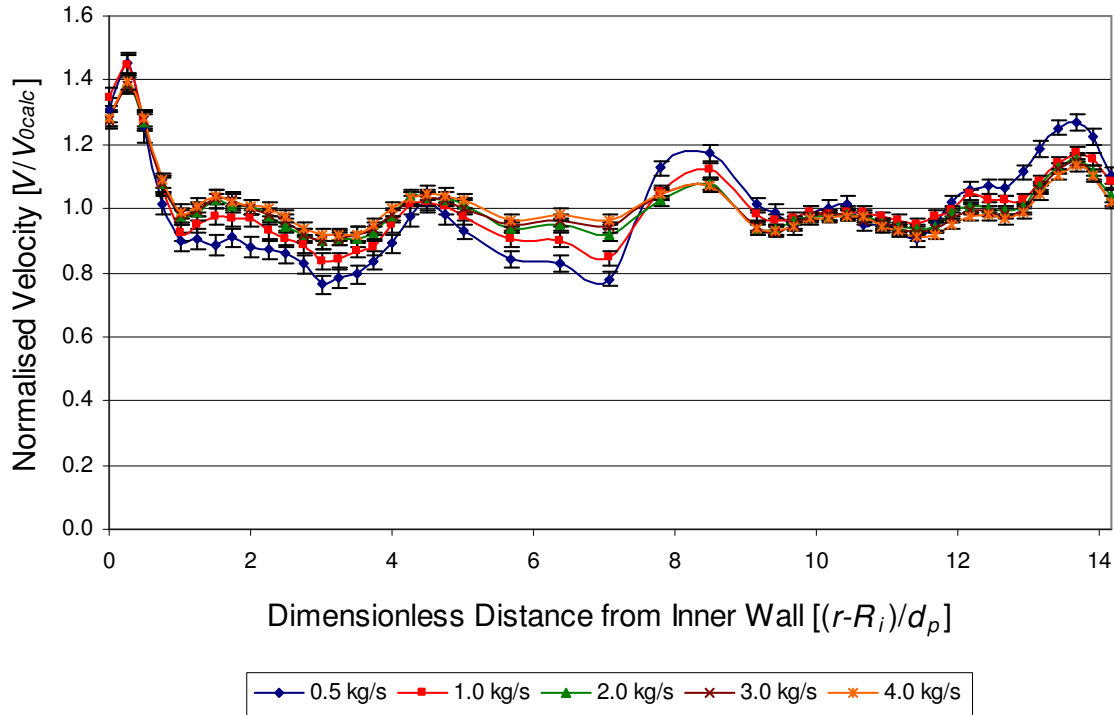


Figure 3-17: Normalized velocity profiles

As seen in Figure 3-17 all the profiles exhibit the same trend. In all the profiles the wall channelling effect is clearly visible near the inner annulus wall. Minor differences in the magnitude of velocity peak near the inner annulus wall, for the different mass flow rates, can be observed. The peak velocity of each profile lies within the uncertainty band of all the other velocity profiles. It can be assumed that the velocity profile is independent for the test's Reynolds number range of $439 < Re < 3453$. The variation between the velocity profiles, at the maximum and minimum mass flow rates, may be attributed to the higher variation/noise in the measurements at the lower mass flow rates. The Reynolds number's independency of the velocity profile corresponds to the findings of Subagyo *et al.* (1997:1383). Subagyo *et al.* (1997:1383) postulated that the velocity profile is independent of mass flow rate for Reynolds numbers larger than $Re > 500$. No difference could be detected between the velocity profiles of Subagyo *et al.* (1997:1383) at Reynolds numbers of $Re = 400$ and $Re = 500$. This indicates that the profile already achieved mass flow independence at a Reynolds number of $Re = 400$. The velocity profiles at $Re = 103$ and $Re = 532$ presented by Giese *et al.* (1998) show very little deviation between the profiles. This enforces the assumption that the velocity profile is independent for the mass flow rate for the Reynolds number range of the HTTU.

Even though wall channelling is observed near the inner annulus wall, this phenomenon isn't clearly visible near the outer annulus wall. A smaller velocity peak, stretched out over a greater radial span is observed near the outer annulus wall. A possible cause for this lies in the geometry of the outer annulus wall and the set-up of the traversing system. As mentioned earlier, the outer annulus wall is not a cylinder but consists of 24 graphite

segments that had been pieced together as shown in Figure 3-4. When the anemometer was traversed at a radius of 1.15 m a majority of the readings would have been taken above the outer reflector wall instead of at the edge of the outer reflector. This is illustrated in the top image of Figure 3-18.

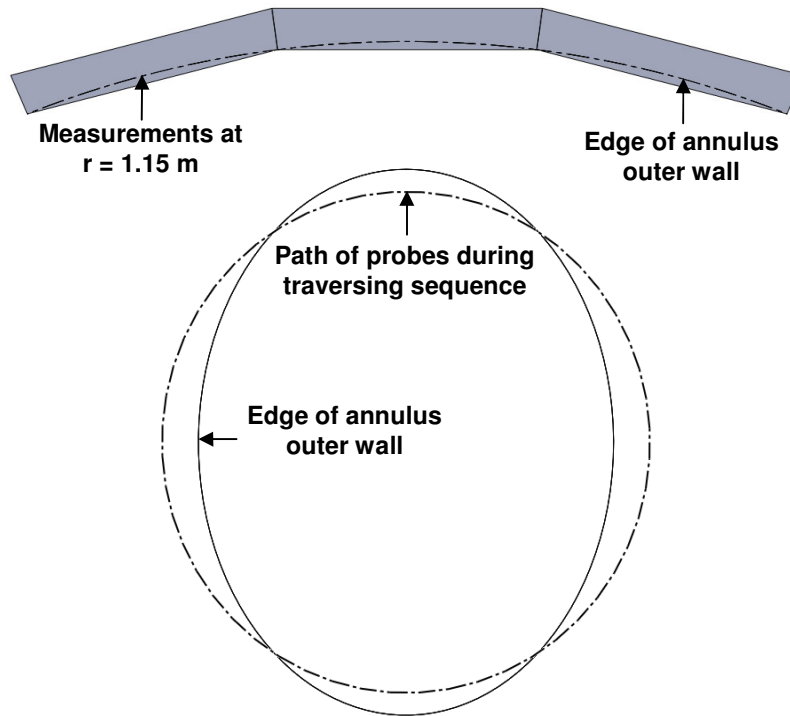


Figure 3-18: Discrepancies in measurements near outer annulus wall

The bottom image in Figure 3-18 also shows that measurements near the outer annulus cannot be classified as a fixed distance from the outer wall due to the oval shape of the wall. At a certain radius some readings will be made closer to the wall while others are made further away from the wall. The velocity peak, near the inner wall, only persists over a small radial span of less than one sphere diameter. The measurements near the outer wall will thus include high (nearer to the wall) and low (further away from the wall) velocity readings. This will cause the profile to be “smeared” near the outer annulus wall explaining the smaller, wider velocity peak and the absence of a prominent velocity peak. The extent of the outer reflector’s oval shape could however not be determined.

Even though there are some discrepancies in the velocity distribution profiles, these profiles provide a good insight into the fluid flow distribution downstream of the bed at a height of 60 mm from the bed.

3.7 Conclusion

This chapter dealt with the experimental procedure that had been used to investigate the velocity distribution above an annular bed packed randomly with spheres. The measuring instruments and set-up thereof was covered in great detail along with the constraints associated with the velocity measurement instruments.

The velocity distribution was investigated at a height of 60 mm above the bed under different mass flow rates corresponding to $439 < Re < 3452$. The shape of the profiles remained constant throughout the Reynolds number range indicating the independence of the profiles on the mass flow rate and Reynolds number. The profiles clearly showed the occurrence of flow channelling near the inner annulus wall. Due to shape and construction method of the outer wall and the measurement process employed, less significant wall channelling was observed near the outer annulus wall. The velocity peak near the inner wall was of order 1.4 times larger than the empty annulus velocity at each mass flow rate and is situated at a distance of $\frac{1}{4} d_p$ from the wall. Integration of the measured velocity profiles indicated a possible error in calibration of the probes at higher mass flow rates. This error seemed to be systematic throughout the entire Reynolds number range and was eliminated by normalising the profiles with the calculated empty annulus superficial velocity. Despite these issues the velocity profiles are good enough to be used in the verification process of the implicit bed simulation model as discussed in chapter 5.

The biggest discrepancy in the velocity measurements is the inclusion of the radial velocity vector component in the measured velocity along with the directional independence of the measurements. This will be the focus of the next chapter where the relation between the axial velocity component and the resultant of the axial and radial velocity components will be investigated by means of an explicit RANS CFD simulation model of a section of the HTTU's annular bed in order to obtain a better understanding of the velocity measurements of the HTTU. Due to the good repeatability between the velocity profiles and the Reynolds number independency of the velocity profiles only the velocity profile obtained during the first test (FCIT1) at a mass flow rate of 0,5 kg/s will be considered from here on onwards.

Chapter 4

Explicit Bed Modelling

4.1 Introduction

This chapter starts with an investigation into the treatment of the contact points between spheres in contact. Lee *et al.* (2007) already demonstrated that the flow field simulation is adversely affected by the manner in which the contact points are modelled. From this investigation a suitable contact point treatment technique is selected and implemented into a simulated section of a randomly packed bed in order to determine the relation between the three velocity vector components in the region downstream of the bed at a specific distance from the bed. This relation will then be compared with the measured velocity profile and serve as a basis to adjust the measured velocity profile to be representative of the axial velocity distribution above the packed bed.

4.2 Simulation of two spheres in contact (CT cases)

4.2.1 Description

Lee *et al.* (2007) already demonstrated that the heat transfer and flow field, in the region downstream of the spheres in contact, are adversely affected by the manner in which the inter-pebble contact regions are modelled. Lee *et al.* (2007) also showed the dependence of the computational mesh size on the contact point treatment technique employed. In cases where the contact points were removed from the model and approximated as gaps the computational mesh size was nearly half the size of the meshes where point and area contact points were included. This is due to the fact that cell sizes need to be drastically reduced in these sharp angled geometry regions around the contact points in order to prevent highly skewed cells being generated resulting in a poor quality mesh. This need for smaller cells near the contact points that cause the model's size, required computational resources and cost to increase drastically. Guardo *et al.* (2005:1736) noted that regions of stagnant flow existed around the contact points. In cases where only the flow and not the heat transfer inside the bed is under investigation these stagnant and low flow regions, around the contact points, may be removed. By removing these stagnant flow regions the size of the mesh is accordingly reduced and will allow for more spheres to be included in the model.

The CT cases were conducted in order to determine how much of the stagnant and low flow fluid region, around the contact points, can be removed without affecting the flow field in the downstream region of the pebbles in contact. The geometry used in the numerical analysis of the CT cases is shown in Figure 4-1.

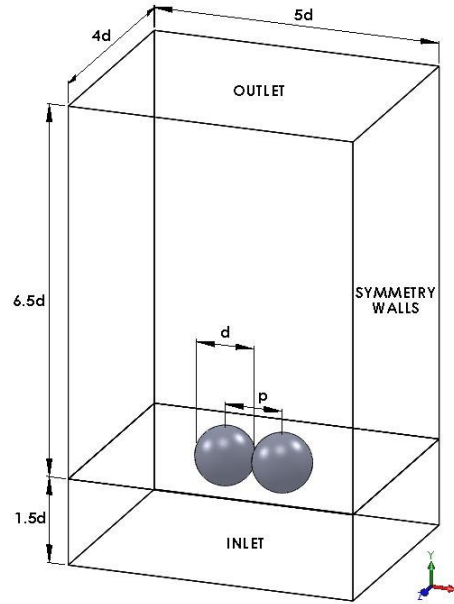


Figure 4-1: CT cases Geometry

Two spheres, in contact with each other, were removed from the numerical model of the HTTU's packed bed, generated by Polson (2008) and used by Du Toit (2008), and aligned horizontally. The diameter of the spheres, d_p , is 60 mm and the contact between them consisted of a contact area, since Polson (2008) included the elastic deformation of the spheres due to the load of the whole packing during the generation of the packed bed. As mentioned previously, the CT cases were conducted in order to determine how much of the fluid region around the contact points can be removed without affecting the flow field to provide guidance to the contact treatment of the packed bed used to investigate the relation between the velocity vector components in the downstream region of the packing as discussed in the following section. Table 4-1 provides a description of the three simulated cases. In CT-1 there was no modification to the contact region between the spheres. In CT-2 and CT-3 cylinders of 5 and 10 mm were removed from the fluid region around the contact points.

Table 4-1: CT cases description

Case	Description	Sphere dia. d_p (mm)	Pitch p (mm)	Contact dia. d_{cont} (mm)	Faces generated on spheres Surface/Volume mesh
CT-1	Area contact	60	59.989	1.149	33762/17874
CT-2	5 mm Area contact	60	59.989	5	30342/16158
CT-3	1 mm Area contact	60	59.989	10	25294/12889

4.2.2 Computational domain, physics models and boundary conditions

In order to investigate the influence the removal of the stagnant and low flow regions has on the flow field, the fluid domain was created as shown in Figure 4-1 with the two touching spheres aligned horizontally with fluid

flowing in the vertical direction over the spheres. Since nitrogen was used during the experimental set-up, the fluid in the simulation was taken as nitrogen at a temperature of 20.107 °C and a pressure of 100.15 kPa which correspond to the conditions during the velocity measurements of FCIT1 at a mass flow rate of 0,5 kg/s.

The computational meshes were generated using the built in meshing tool of STAR-CCM+®. The same approach as Calis *et al.* (2001) was used in the generation of the computational mesh. The first couple of cell layers adjacent to the pebble wall consisted of structured prismatic cells (prism layer) while the remainder of the mesh was unstructured and consisted of polyhedral cells. The prism layer thickness was confined to 2 mm and consisted of two prismatic cell layers. The thickness of these individual layers was scaled by a ratio of 1.5. A maximum and minimum cell size of 4.0 and 0.1 mm was chosen. These values give a sphere diameter to cell size ratio of $d_p / C_{s-\max} = 15$ and $d_p / C_{s-\min} = 600$ which is in line with the ratios used by other researchers (Calis *et al.*, 2001; Tobis, 2000; Wang-Kee In & Hassan, 2008). A surface growth rate of 1.3 was used in the generation of the surface mesh. The resulting number of faces created on the pebble's surfaces is shown in Table 4-1. Due to the removal of the high angled geometry region around the contact points the surface mesh required less faces to fully define the sphere geometry and ultimately reduces the number of cells in the computational volume mesh.

Since no significant differences between the various turbulence models, in their applicability to packed beds, could be identified it was decided to use the $k - \varepsilon$ turbulence model since its the most commonly used model. For the wall treatment, the two-layer wall treatment model with the realizable $k - \varepsilon$ turbulence model was used. The fluid domain was taken as stationary while the fluid flow was assumed to be steady. The fluid was assumed to be an ideal gas.

The boundaries used in the CT case simulations include a velocity inlet, a pressure outlet, walls and symmetry wall. For the velocity inlet a uniform velocity (V_0) of 0.1122 m/s was specified, which corresponds to a mass flow of 0.5 kg/s through an empty annulus with an outside and inside radius of 1.15 m and 0.3 m. The relative pressure of the pressure outlet was set to 0 Pa. This pressure is relative to a pressure of 100.15 kPa. For both the inlet and outlet reverse flow a turbulence intensity of 5% was specified. The pebble surfaces were treated as smooth, no-slip walls.

For the CT case simulations the simulation was deemed as converged if the residuals reached a steady value and preferably reached a value smaller than 10^{-3} . All the residuals except the energy residual met these criteria. A possible explanation for this is the fact the simulation tried to achieve a steady state solution to a problem that is transient.

4.2.3 Results and discussion

A comparison of the results for each of the three CT cases is shown from Figure 4-2 to Figure 4-7. The results are shown on vertically aligned planes through the centre of the contact point (mid plane) between the spheres at $X = 0$ and $Z = 0$. The colour contours and values in each of the results plots are based on the range of data for each individual case.

The pressure distribution for all three CT cases is shown in Figure 4-2. In all three cases the position of the maximum and minimum pressure is the same namely the maximum pressure is observed at the bottom of the spheres while the minimum pressure is observed at the outer parts of the spheres due to the curvature. The magnitude of the predicted maximum and minimum pressure is also in good agreement between the three cases, with a maximum difference of 0.12% in predicted maximum pressure between CT-1 and CT-2 and a difference of 2.75% in the predicted minimum pressure between CT-1 and CT-3. Minor differences can also be observed downstream of the pebbles.

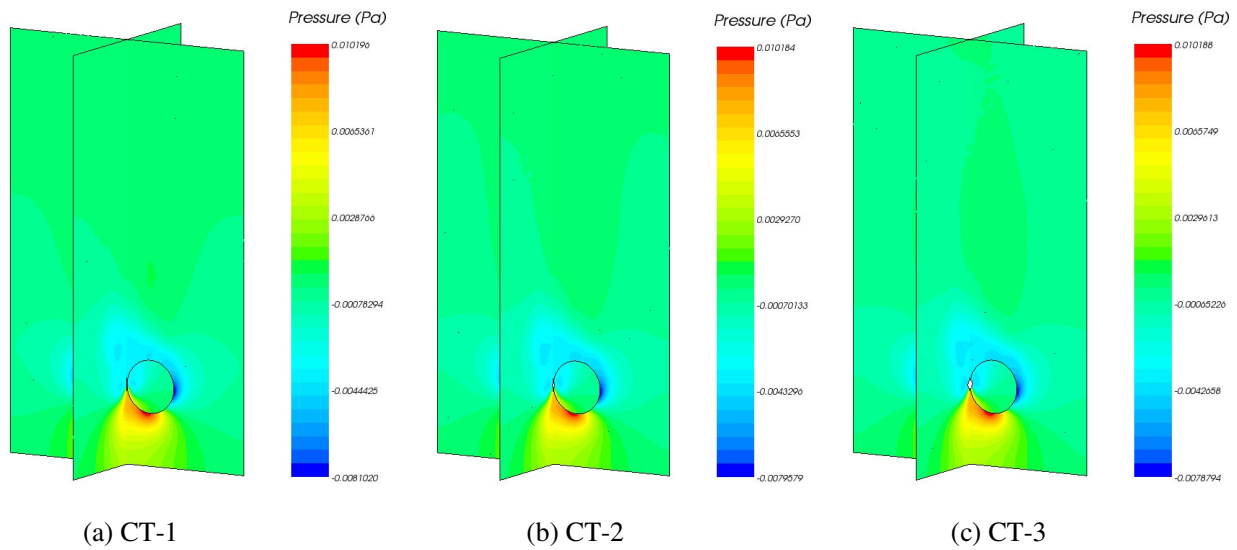


Figure 4-2: Pressure distribution on mid planes for CT cases

A comparison of the velocity distribution for the three cases is shown in Figure 4-3. All three cases yield basically the same results with the maximum predicted velocity differing between CT-1 and CT-2 by 0.49%.

The vorticity and turbulent kinetic energy plots are shown in Figure 4-4 and Figure 4-5. As with the velocity distribution, a comparison between the three cases shows very little difference between one another. This implies that the removal of the stagnant flow regions did not induce extra swirl and turbulence into the flow field.

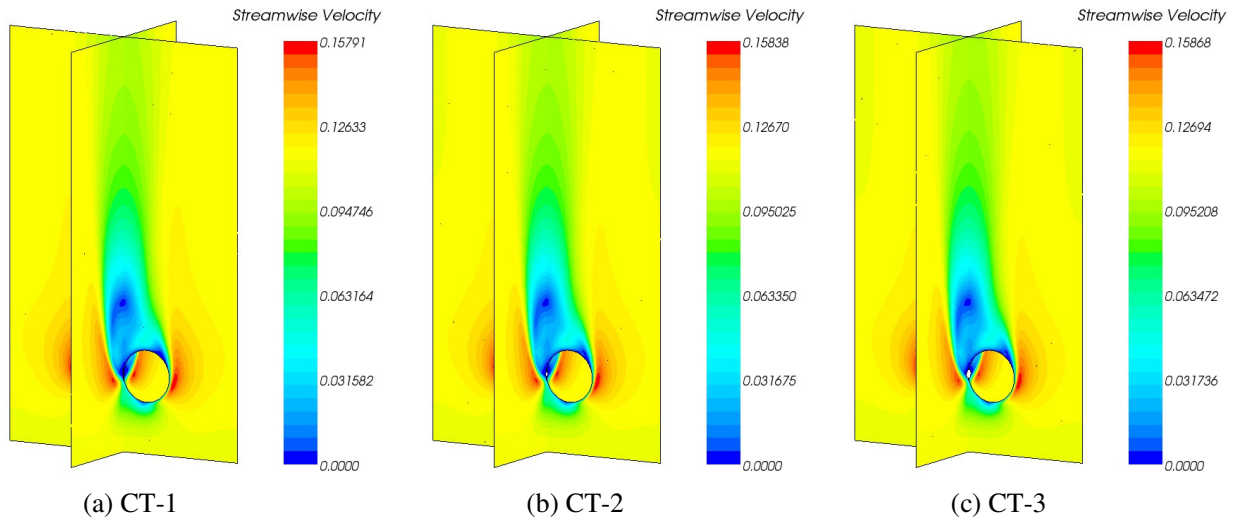


Figure 4-3: Velocity distribution on mid planes for CT cases

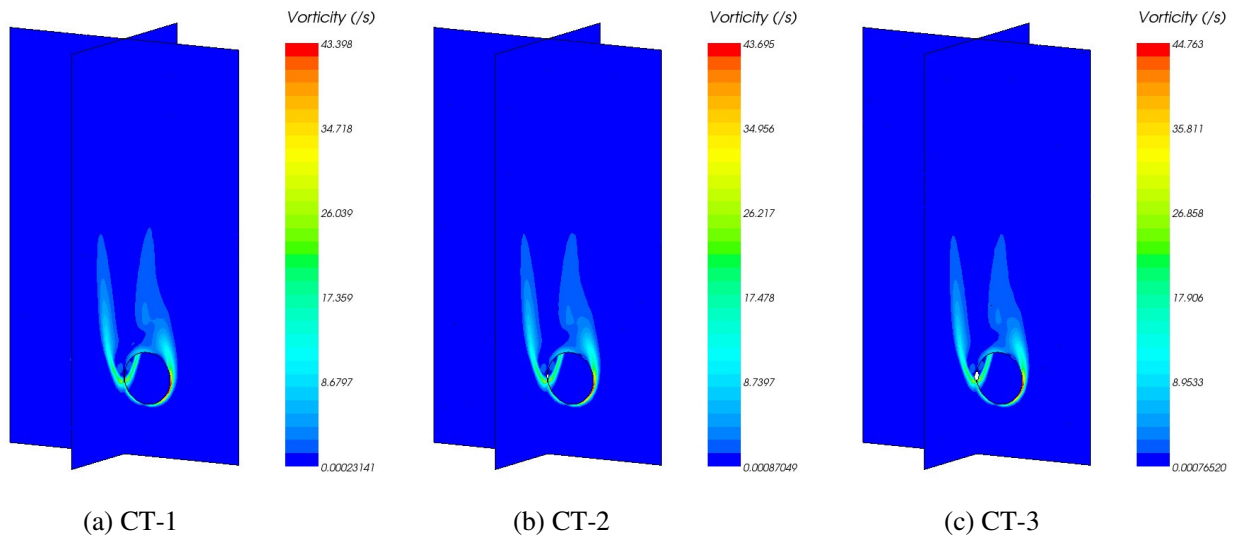


Figure 4-4: Vorticity distribution on mid planes for CT cases

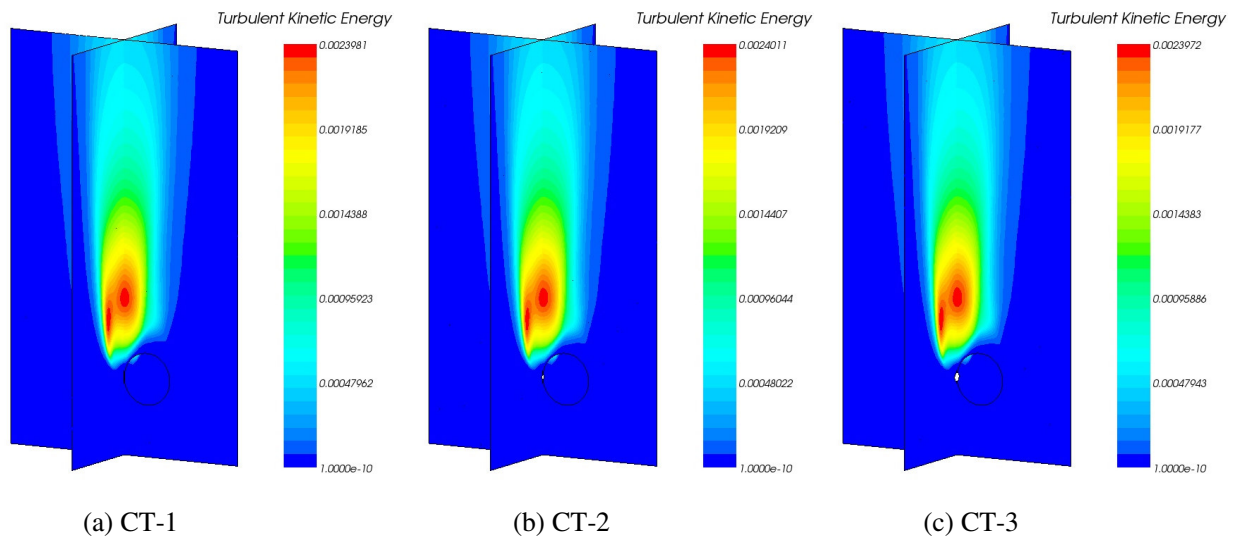


Figure 4-5: Turbulent kinetic energy distribution on mid planes for CT cases

The comparison of the pressure distribution on the surface of the spheres is shown in Figure 4-6. The pressure distribution on the bottom and side of the spheres is almost identical in all three cases. The pressure distribution on top of the spheres differ somewhat. In the cases where the contact point was modified, by removing the stagnant flow region from the computational mesh (CT-2 and -3), the pressure on top of the spheres seems to be a small amount lower than the case where no modification was done (CT-1). If one looks at the streamline shown in Figure 4-7 it can be seen that the regions where the pressure distribution differs coincides with the region where vortices are formed at the rear of the spheres. This difference may be the effect of stronger vortices being formed at the rear of the spheres in cases CT-2 and CT-3 where the stagnant flow regions were removed. By looking at the scale of pressure distribution is clear that the differences are however negligible.

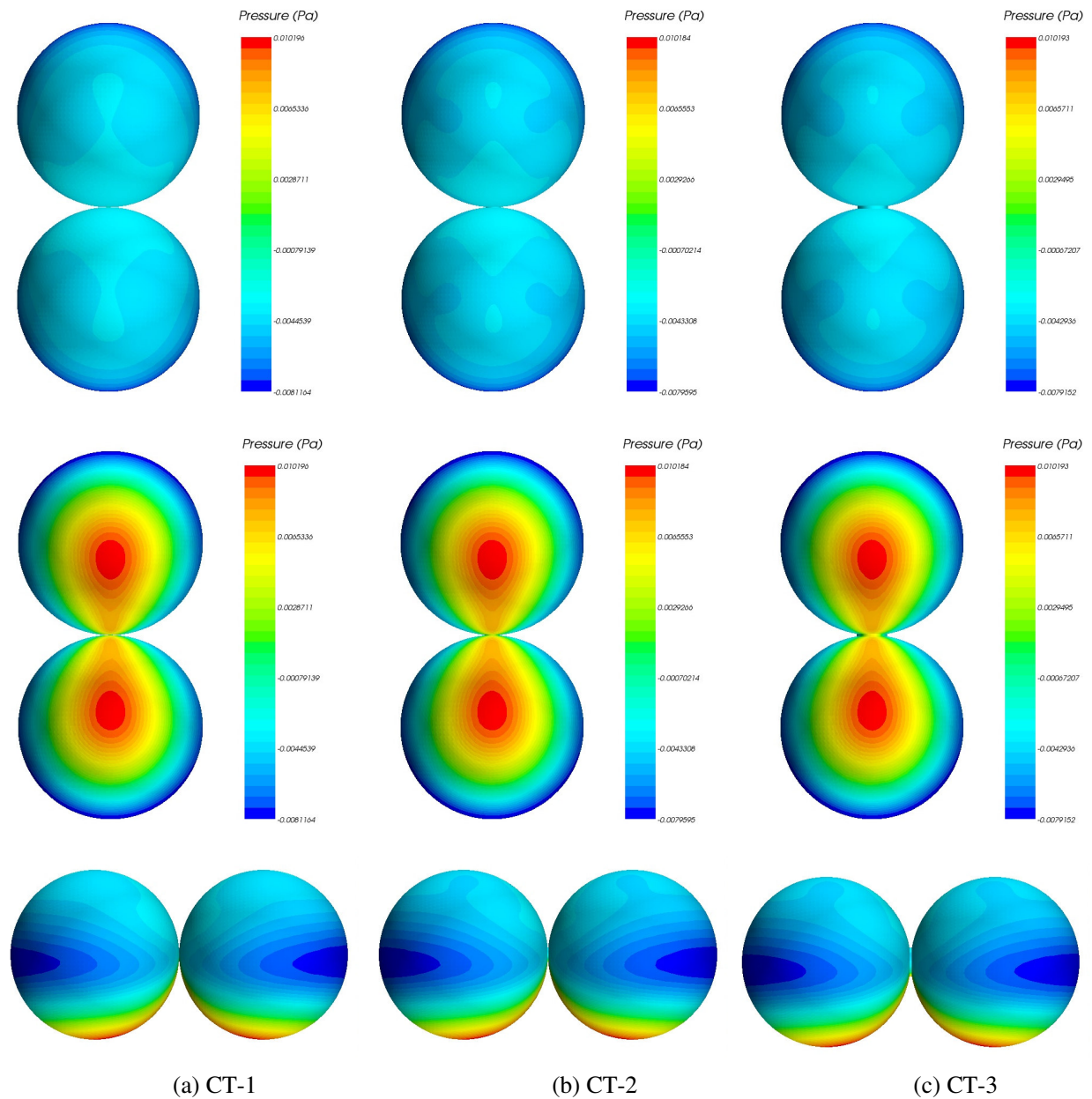


Figure 4-6: Pressure distribution on sphere surface projected from the top (upper) the bottom (middle) and the side (lower)

The streamlines for all three cases are shown in Figure 4-7. As seen from the lower figures in Figure 4-7, four vortices are formed at the rear of the spheres. In all three cases the differences between the streamline profiles are negligibly small. The velocity magnitude is overlain on the streamlines and little to no difference can be observed between the three cases.

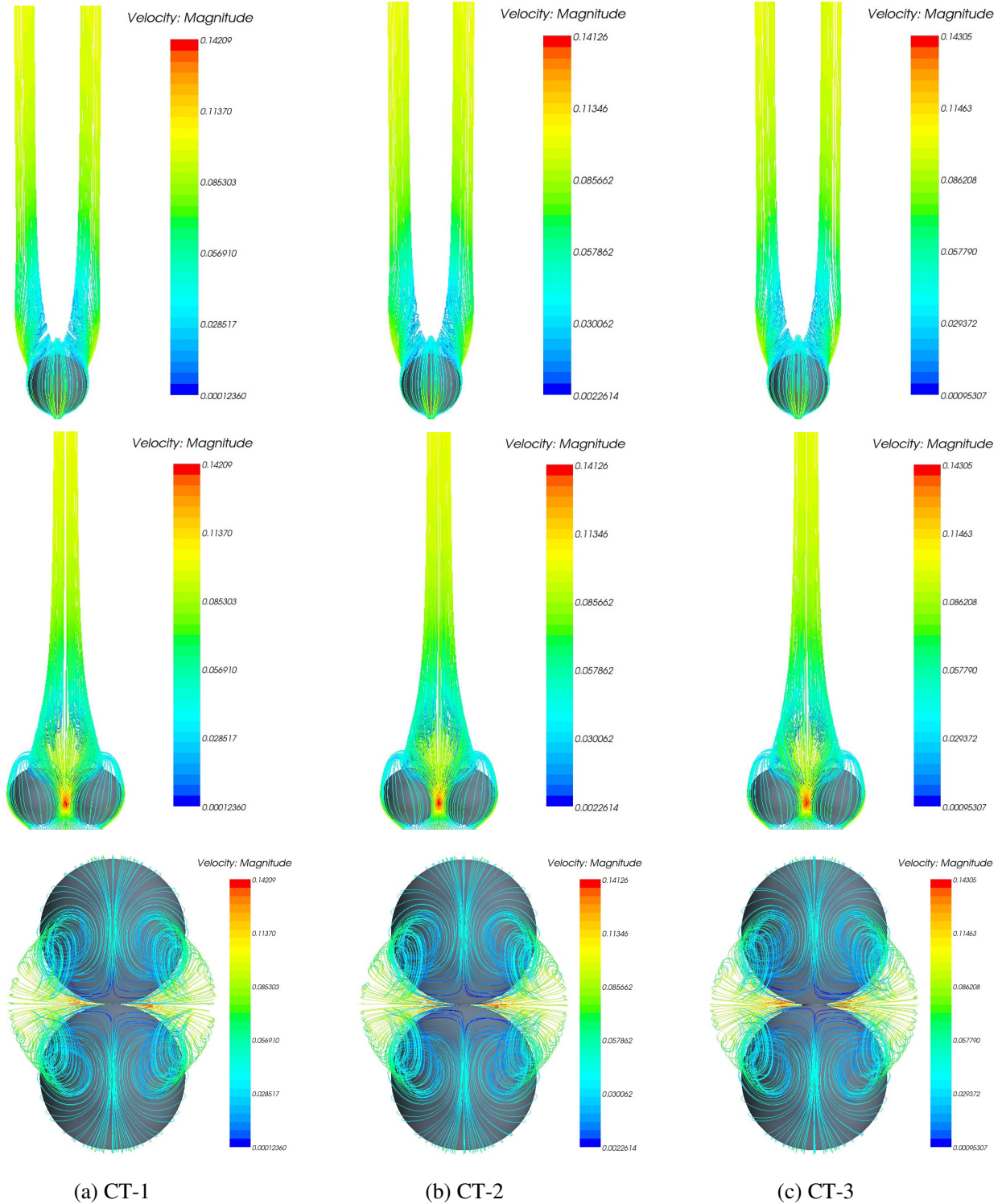


Figure 4-7: Streamlines downstream of the spheres projected from the X-direction (upper) the Z-direction (middle) and the Y-direction (bottom)

From these results it is clear that the removal of the stagnant and low flow regions around the inter-pebbles contact region has little to no effect on the fluid flow downstream of the pebbles. A 10 mm cylinder of fluid can thus be removed around the contact point without disrupting the fluid flow in larger packings of spheres in order to reduce the computational resource requirements, computational time and to allow for more spheres to be included in the simulation model.

4.3 Simulation of a randomly packed bed (VM case)

4.3.1 Description

Since a single sensor hot-wire anemometer was used during the velocity measurements it was impossible to measure only the axial velocity distribution since the probe can only measure the velocity component perpendicular to the probe's wire. Another shortcoming of the probe is that the measurements are direction independent, meaning that probe cannot detect whether measured velocity is positive (flow out of the bed) or negative (reverse flow into the bed). During the set-up of the probe, it was orientated in such a way that the probe wire was tangent to the curvature of the annulus. This implied that the probe measured the resultant of the axial and radial velocity components. These shortcomings of the probe could be seen when the measured velocity profile was integrated over the entire annular region. This integration yielded a volume flow rate that was converted to a mass flow rate. The calculated mass flow rate, for FCIT1, was 27.25% higher than the actual input mass flow rate due to the errors in measurement. The VM case was thus conducted to investigate the relation of the axial velocity component to the resultant of the axial and radial velocity components downstream of a packed bed at a certain distance from the bed. The geometry of the VM case can be seen in Figure 4-8 while the values of the geometric parameters are given in Table 4-2

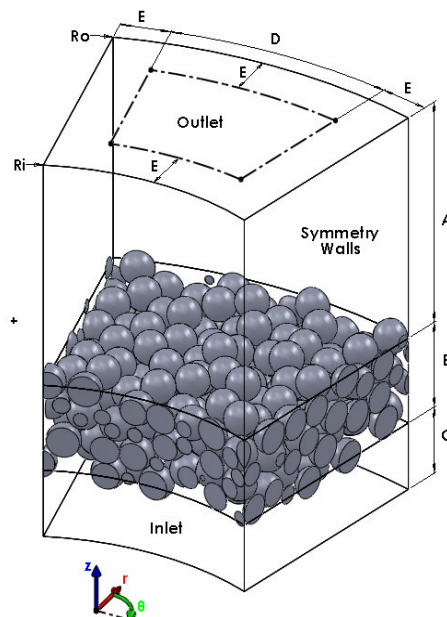


Figure 4-8: VM case geometry

Table 4-2: Geometric parameters of VM case

Parameter	Description	Value
A	Distance from highest pebble centre to outlet	431.5 mm
B	Distance from highest pebble centre to lowest pebble centre	130 mm
C	Distance from lowest pebble centre to inlet	166.1 mm
D	Pie segment of valid fluid flow region	24°
E	Distance from valid fluid region to symmetry walls	90 mm
R _i	Inner radius	510 mm
R _o	Outer radius	940 mm

4.3.2 Computational domain, physics models and boundary conditions

In order to get a good indication of the relation between the axial velocity component and the resultant of the axial and radial velocity components it was decided to use packing that is only a few pebbles high and has a relatively large surface area. The computational domain was limited to the central part of the annulus with a maximum outer radius of 940 mm and a minimum inner radius of 510 mm. Only 1/15th of this annular ring was analysed. Since symmetry wall conditions would enclose the computational domain, the symmetry walls were offset by a distance of $1.5 d_p$ from the region of interest, in order to minimize the effect the symmetry walls could have on the fluid flow. All the pebbles falling within these bounds were extracted from the numerically packed bed of Polson (2008). From this selection the first 250 spheres, whose centres were not higher than 1170 mm from the bottom-containing wall, were removed. Contact points between spheres were treated as described in Section 4.2 by means of a 10 mm cylinder. The geometry of the final computational domain can be seen in Figure 4-8 and contained 142 uncut, 108 partially cut spheres and 483 contact points.

The computational domain was once again meshed using the built in mesher of STAR-CCM+®. For the inlet, outlet and symmetry walls a target and minimum cell size of 6 mm and 2 mm was specified. In order to achieve a finer mesh on the surface of the pebbles a target and minimum cell size of 4 mm and 0.3 mm was specified. This yielded pebble diameter to cell size ratios of $d_p / C_{s-\text{tar}} = 15$ and $d_p / C_{s-\text{min}} = 200$. These ratios are in line with ratios used by Calis *et al.* (2001), Tobis (2000) and Wang-Kee In and Hassan (2008). The computational mesh consisted of a mixed structured and an unstructured mesh. The structured grid was generated adjacent to the pebble surfaces and consisted of two layers of prismatic cells. These prism layers were grown at a rate of 1.5 and the final combined thickness was set to 2 mm. The unstructured mesh, consisting of polyhedral cells, was then grown from the structured mesh. To ensure that a high quality mesh was generated, automatic mesh refinement was employed. The results of the automatic mesh refinement can be seen in Figure 4-9 as the mesh density is increased around the contact points and on regions of the pebbles that is in close proximity to another pebble.

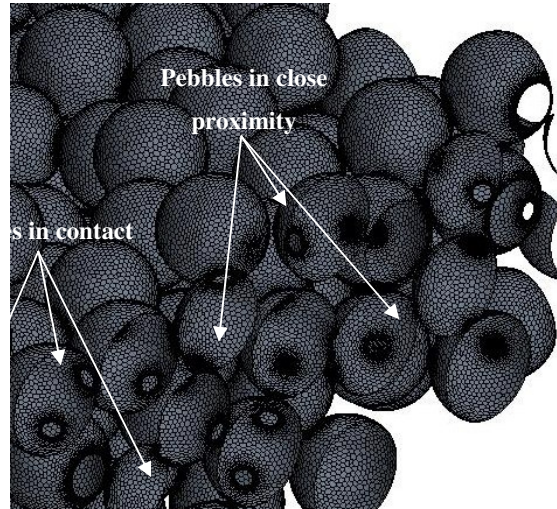


Figure 4-9: Mesh density on pebbles

The fluid in the model is once again taken as nitrogen at a temperature and reference pressure of 20.107 °C and 100.15 kPa, which corresponds to the conditions of FCIT1 at a mass flow rate of 0,5 kg/s. The fluid was modelled as an ideal gas, with the flow being steady and three-dimensional. The fluid flow regime is also assumed to be turbulent since the Reynolds number (based on particle diameter and interstitial velocity $(V_0 / \bar{\varepsilon})$) is $Re_{inter} \approx 1124$ and according to Hlushkou and Tallarek (2006:83) the flow is turbulent when $Re_{inter} \geq 500$. The $k - \varepsilon$ turbulence model is once again employed. Due to the complex geometry inside the packing and high interstitial velocities the high $y+$ wall treatment technique with realizable- $k - \varepsilon$ turbulence model was used to resolve the boundary layer on the pebble surfaces.

The inlet to the fluid domain was modelled as a velocity inlet with the uniform velocity distribution of magnitude 0.1122 m/s at a temperature of 20.107 °C. The outlet of the fluid domain was modelled as a pressure outlet with a relative pressure of 0 Pa. This pressure is relative to a pressure of 100.15 kPa. For both the in- and outlet boundaries a turbulence intensity of 5% was specified. The pebble surfaces were treated as smooth, no-slip walls.

The simulation model would be validated by means of the pressure drop across the packing. The region over which the pressure drop will be validated is shown in Figure 4-10. The entrance of the “Valid Pressure drop Region” is situated 30 mm above the centre of the lowest pebble in the packing in order to allow the uniform velocity distribution to develop before entering the “Valid Pressure drop Region”. The exit of the “Valid Pressure drop Region” is situated 30 mm below the centre of the highest sphere.

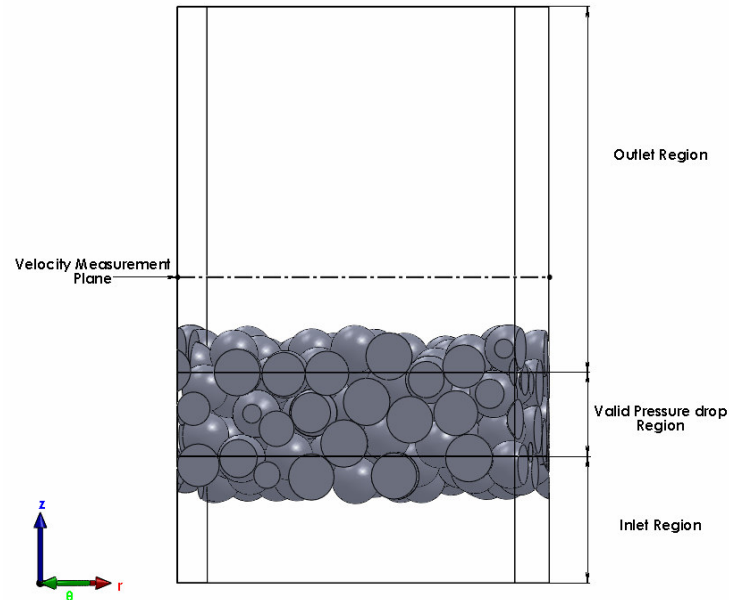


Figure 4-10: Definition of valid pressure drop region and velocity measurement plane

Figure 4-10 also shows the plane on which the velocity components were measured. This plane was situated 90 mm above the centre of the highest sphere in the packing. This corresponds to a measurement height of 60 mm from the bed and was in accordance with the measurement height above the bed during the actual velocity tests. The velocity components were measured by means of “line probes” containing 51 equally spaced measurement points. In total, 51 of these line probes were used and were evenly spaced out in the tangential direction. As stated previously no measurements were taken in regions closer than 90 mm from the symmetry walls. The layout of the measurement points is shown in Figure 4-11.

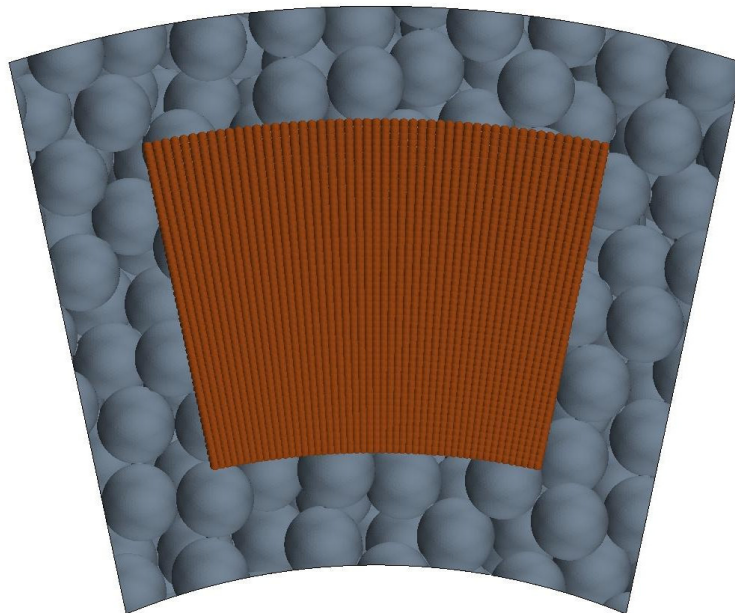


Figure 4-11: Velocity measurement positions

The simulation was deemed as converged once the residuals reached a steady value smaller than 10^{-3} . The mass flow at the inlet and outlet of the packing was used as an additional convergence monitor and should also reach a steady value.

4.3.3 Results and discussion

The theoretical pressure drop over the “Valid Pressure drop Region” is provided by the KTA (1981) pressure drop correlation (2.18). The porosity ($\bar{\varepsilon}$) of the “Valid Pressure drop Region” was calculated as $\bar{\varepsilon}_{cm} = 0.3898$ (contact point modification included) and $\bar{\varepsilon}_{ncm} = 0.3903$ (contact point modification excluded). The density (ρ) and dynamic viscosity (μ_f) of nitrogen, at a pressure and temperature of 100.15 kPa and 20.107 °C, was determined with EES (Engineering Equation Solver) as $\rho = 1.150924 \text{ kg/m}^3$ and $\mu_f = 1.79069 \times 10^{-5} \text{ kg/m} \cdot \text{s}$. The “Valid Pressure drop Region” had a bed length (L) of 0.106081 m. Using these values, the theoretical pressure drop over the packing is given in Table 4-3.

Table 4-3: Theoretical pressure drop over packing

<i>Description</i>	<i>ΔP (Pa)</i>
Bed with modified contact points	0.4702
Bed without modified contact points	0.4680

The simulated pressure drop was predicted as 0.4765 Pa. This is in excellent agreement with the theoretical pressure drop. The simulated and theoretical pressure drop, for the bed containing contact point modifications, differ by 1.32% while a difference of 1.82% is observed between the simulated and theoretical pressure drop for the packing containing no contact point modifications.

Figure 4-12 and Figure 4-14 show the flow field results of the simulation. The upper part of Figure 4-12 shows the velocity vector plot on the plane of measurement with the pebbles visible. The flow is completely random. Multiple regions of high fluid flow can be observed and these regions tend to correspond to less dense regions in the packing. The maximum velocity observed is an order of 7.13 larger than the input velocity. Several vortices can also be identified in the flow field and these are more clearly visible in the lower part of Figure 4-12.

The velocity distribution above the annular bed, generated from the physical experimental data, can be seen in Figure 4-13. During the actual experiment, the maximum observed average velocity was 0.38 m/s. This is significantly lower than the maximum predicted in the simulation. It should however be remembered that Figure 4-13 show the average velocity distribution, calculated from 60 measurements, per point. The velocity measurements contained a significant amount of noise and the averaging of the 60 velocity readings may thus

cause the average point velocity to be lower than the maximum measured velocity in the 60 readings. The maximum point velocity observed, for the central part of the annulus during the physical experiment, was 0.608 m/s, which is only 20% lower than that observed in the simulation. Further more, the high velocity regions, shown in Figure 4-12, are very small (less than a particle diameter) and the measurement grid, used during the physical experiments, is quite coarse so it would have been easy to “miss” these small high velocity regions during the experiment.

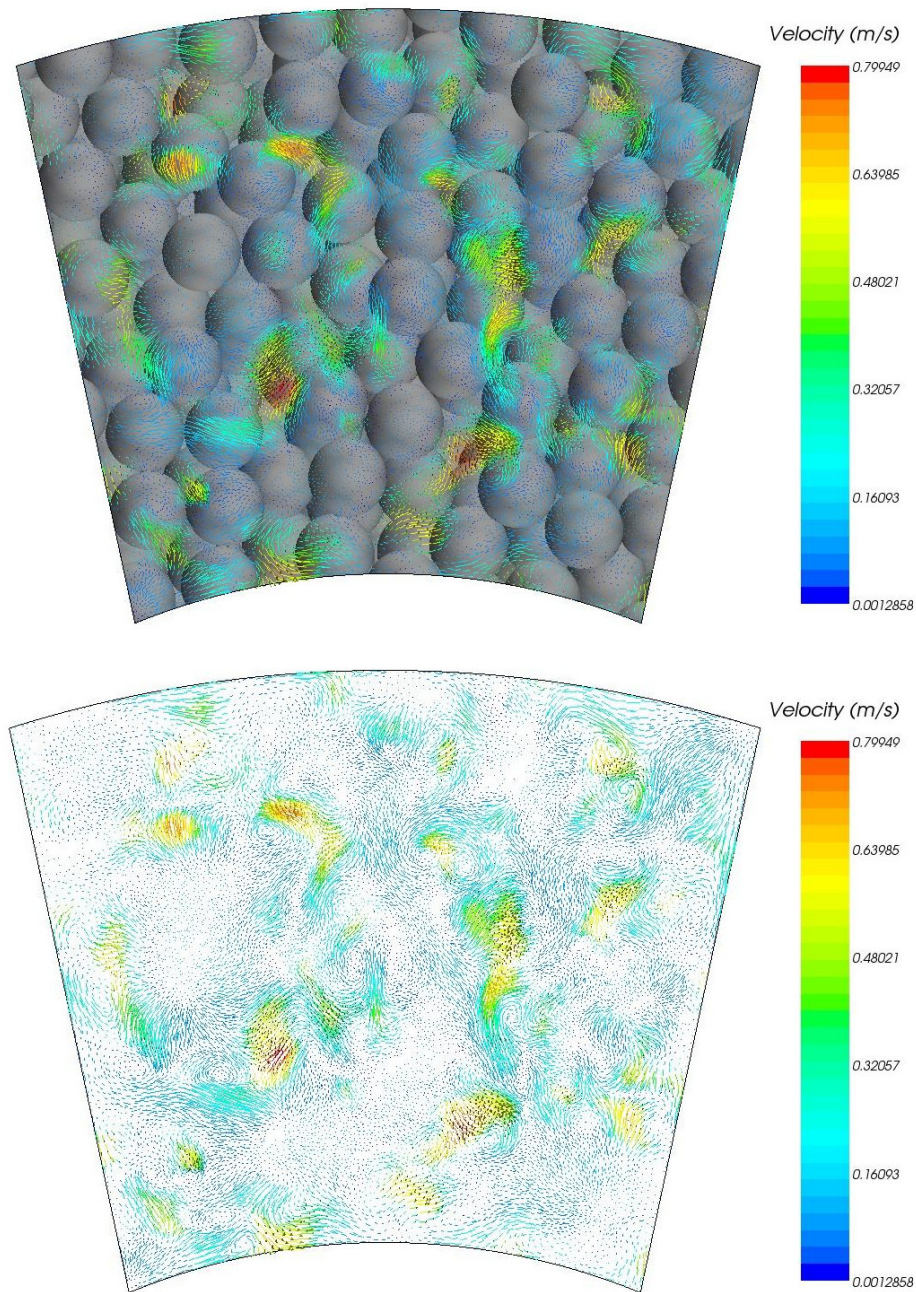


Figure 4-12: Velocity vectors with (upper) and without (lower) pebbles visible

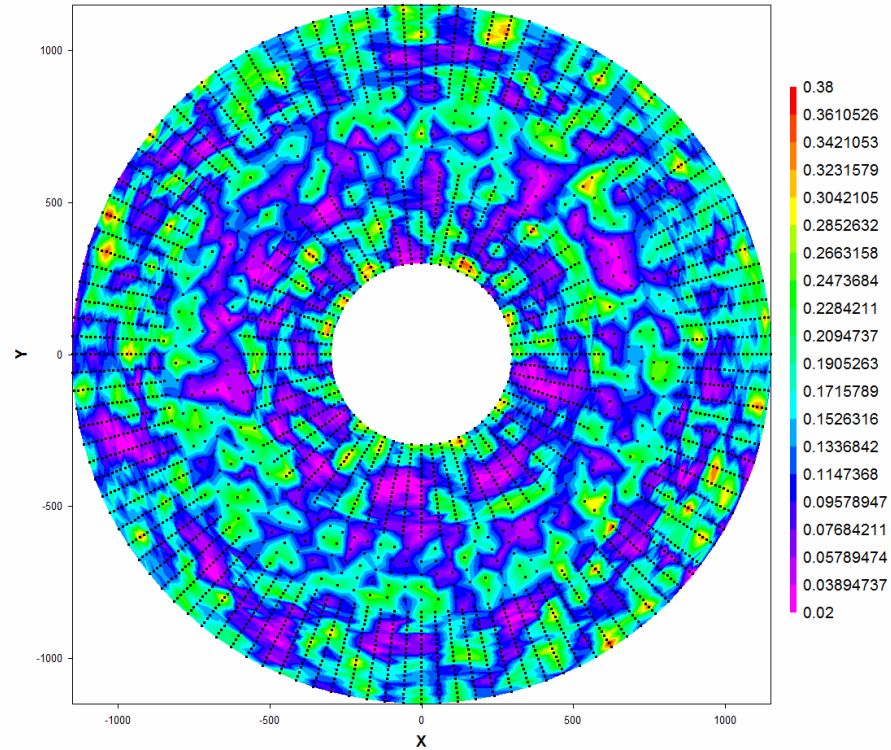


Figure 4-13: Experimental velocity distribution above annulus

It can thus be concluded that the simulated velocity distribution is representative of the measured velocity distribution present during the physical experiments. From the vector plots it is also clear that the measured velocity profile does not represent the axial velocity distribution above the annular packed bed but rather the resultant of the axial and radial velocity components.

Figure 4-14 shows the distributions of the various velocity vector components on the entire plane of measurement. As seen from the upper images in Figure 4-14, the average radial and tangential velocity components is close to zero even though a couple of high velocity regions are observed. From the axial velocity distribution it is interesting to see that there exist quite a few regions of reverse flow back towards the bed. By comparing the axial velocity component distribution with the pebble positions, shown in the upper part of Figure 4-12, it can be seen that most of these reverse flow regions are directly above the highest spheres in the packing. These negative flows would have been perceived as positive by the hot-wire probe and will also induce an error in the velocity measurements.

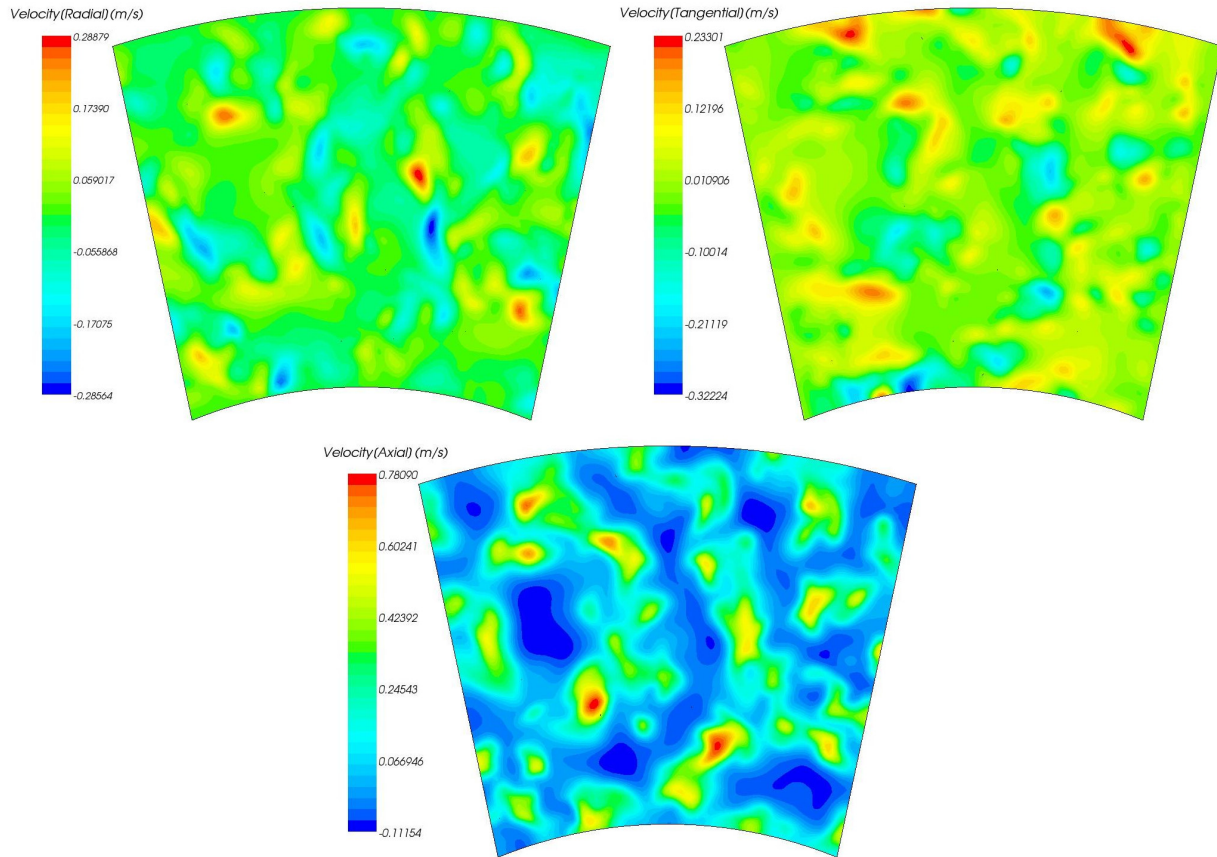


Figure 4-14: Velocity vector components (upper left: radial, upper right: tangential & lower: axial)

As mentioned earlier, a total of 2601 measurements of the radial, tangential and radial velocity components were made. For each point the resultant, of the radial and axial velocity components, was calculated. The average values of the radial, tangential, axial and the resultant of the axial and radial velocity components are given below in Table 4-4

Table 4-4: Average Velocity Components

Description	Value (m/s)
Average Radial Velocity Component ($\overline{V_{0r}}$)	-0.007256
Average Tangential Velocity Component ($\overline{V_{0\theta}}$)	-0.003070
Average Axial Velocity Component ($\overline{V_{0z}}$)	0.114391
Average Resultant of Axial en Radial Velocity Components ($\overline{V_{0reslt}}$)	0.142802

If the average axial velocity component ($\overline{V_{0z}}$) is written as a percentage of the average resultant ($\overline{V_{0reslt}}$), it is found that:

$$\overline{V_{0z}} = 0.801 \overline{V_{0reslt}} \quad (4.1)$$

It is thus possible to calculate the average axial velocity component from (4.1) provided the average resultant of the axial and radial velocity components are known.

All the simulation files are provided on the first disk at the back of the thesis.

4.4 Velocity profile adjustment

Since the hot-wire anemometer was positioned in such a way that it measured the resultant of the axial and radial velocity components, equation (4.1) can now be used to extract the axial velocity distribution profile from the measured velocity profile if it is assumed that equation (4.1) is also valid in the near wall regions. Figure 4-15 shows a comparison between the measured and adjusted velocity profiles.

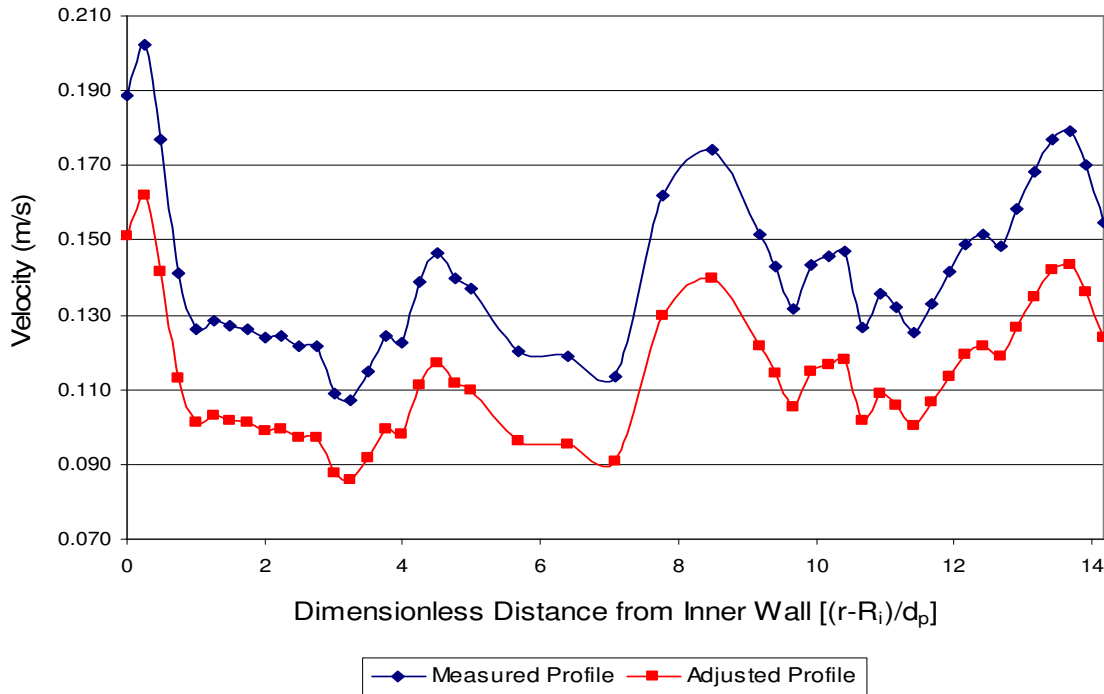


Figure 4-15: Comparison between measured and adjusted velocity profile

The integration of the adjusted velocity profile, over the entire region of the annulus, yields a mass flow rate of 0.5097 kg/s that differs from the actual mass flow rate of 0.5 kg/s by 1.93%. The adjusted velocity profile can thus be assumed to be descriptive of the axial velocity distribution above the bed at a distance of 60 mm from the bed and will be used in verifying the implicit model of the HTTU's packed bed.

4.5 Conclusion

In this chapter it was shown that the removal of the stagnant and low flow regions between touching spheres did not affect the flow field downstream of the pebbles. The modifications made to the contact points also resulted in a computational mesh with a smaller cell count. This in turn reduced the computational resources required, computational cost and time. This contact treatment technique was implemented into a simulation of a randomly packed bed of spheres. From this simulation it was deduced that a factor of 0.801 of the resultant of the axial and radial velocity components represents the axial velocity component at a height of 60 mm from the packing at a mass flow rate of 0.5 kg/s. This factor was used to extract the axial velocity distribution from the measured velocity profile of FCIT1. The axial/adjusted velocity profile will be used in the verification of the implicit bed model, describing the velocity distribution inside the packed bed, in the next chapter.

Chapter 5

Implicit Bed Modelling

5.1 Introduction

This chapter focuses on the development of a mathematical model that is capable of predicting the superficial velocity distribution inside an annular bed with randomly packed spheres. As mentioned in Chapter 2, most models, where the presence of the pebbles is modelled implicitly, only describe the velocity distribution at a distance inside the bed where the flow can be assumed to be fully developed. They do not provide any information regarding the fluid flow development in the in - and outlet regions of the bed. This is partly due to the fact that no correlation exists which predicts the structure of the bed in these regions. The chapter starts off by investigating an adequate manner in which the axial and radial porosity correlations can be combined to describe the structure of the bed in these regions of interest. This appropriate approximation of the porous structure is then applied to a series of fluid flow simulations through the implicitly modelled annular bed of the HTTU. These simulations address uncertainties regarding what porosity correlation and effective viscosity model yields a velocity distribution similar to that, which had been obtained experimentally. The chapter concludes with an investigation into the fluid flow distribution through an implicitly modelled annular packed bed using the verified modelling methodology. Of special interest is the velocity profile development through the inlet region of the bed, the fully developed velocity profile inside the bed and the fluid flow redistribution through the exit region of the packed bed.

5.2 Packing Structure

5.2.1 Description

In simulation models where the spheres and pores are modelled implicitly, the structure of the bed is represented by an empirical porosity correlation. These correlations describe the variation of porosity in either the axial or radial direction. These correlations do however not predict the porosity distribution in the inlet and outlet regions of the bed. These regions of interest are shown graphically in Figure 5-1.

Because the velocity measurements were taken downstream of the bed it is of utmost importance to accurately simulate the fluid redistribution, which occurs in the outlet region of the packed bed.

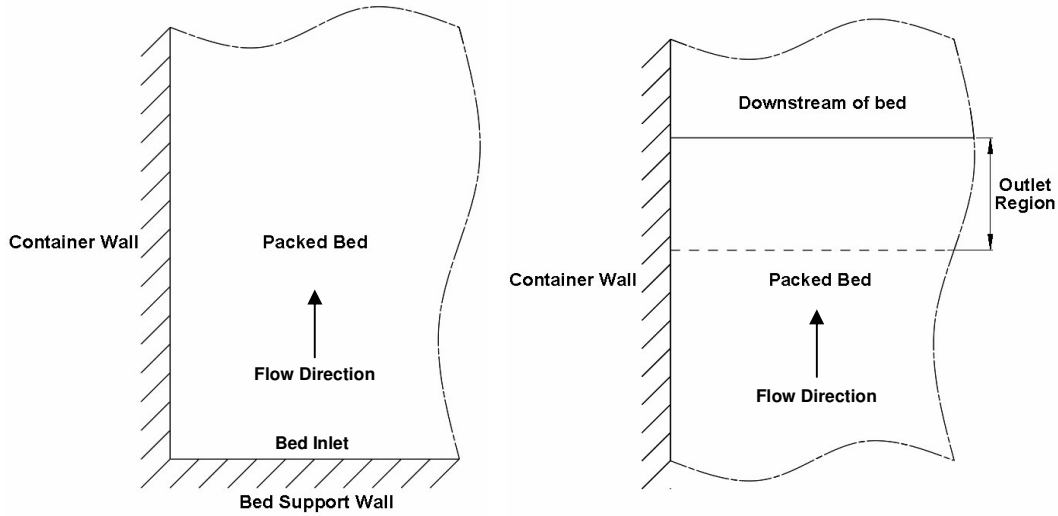


Figure 5-1: Regions of unknown bed structure (inlet (left) and outlet (right))

From the axial porosity variation graphs, presented by Du Toit (2008), it seemed as though the porosity increases linearly to unity over a distance of one particle diameter in the bed outlet region. It was therefore decided to let the porosity, in the outlet region, increase linearly to unity from the porosity predicted by the radial porosity correlation.

As the porosity at a certain point in the packing can only be a single value, there must therefore be a certain relation between the correlations representing the axial and radial variation in porosity. Goodling *et al.* (1983:29) found that for cylindrical packed beds, consisting of uniformly sized spheres, the oscillation in porosity can be detected as far as five sphere diameters from the containing wall. This region is thus confined to a distance smaller than 5 sphere diameters from both the support and container wall as seen in Figure 5-2. Since two walls are present in the inlet region it was decided that the porosity in this region would be best described as a weighted average of both the axial and radial porosity distributions, which is dependant on the distances from the particular walls.

5.2.2 Mathematical formulation

The porosity distribution for the outlet region was approximated as:

$$\varepsilon(r, z) = \left(\frac{1 - \varepsilon(r)}{d_p} \right) z + \left(1 - \left(\frac{1 - \varepsilon(r)}{d_p} \right) L \right) \quad \text{for } L - d_p < z \leq L \quad (5.1)$$

where $\varepsilon(r)$ is the radial variation in porosity given by either equation (2.6) or (2.9), r and z are the radial and axial coordinates of the point under consideration.

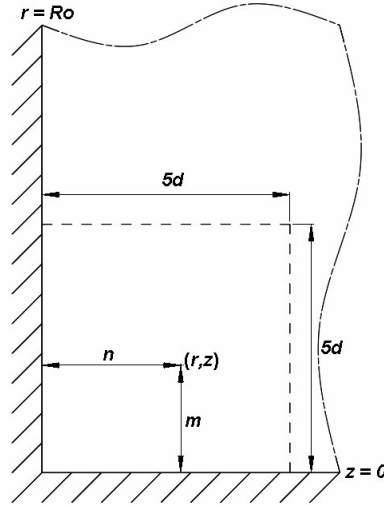


Figure 5-2: Weighted average region in packing inlet

For the region in the inlet, enclosed by the dashed line as shown in Figure 5-2, the porosity distribution was approximated as:

$$\varepsilon(r, z) = \frac{(5d_p - n)\varepsilon(r) + (5d_p - m)\varepsilon(z)}{(5d_p - n) + (5d_p - m)} \quad \text{for } m < 5d_p \text{ \& } n < 5d_p \quad (5.2)$$

where $\varepsilon(r)$ is the radial variation in porosity given by either equation (2.6) or (2.9), $\varepsilon(z)$ is the axial variation given by adapting either equation (2.6) or (2.9) to be dependant on the distance from the bottom support wall and not the container wall, n and m is the distance from the particular walls as shown in Figure 5-2.

5.2.3 Numerical porosity investigation

In order to verify the methodology used to model these regions of unknown bed structure, the porosity of similar regions in the numerically packed bed of the HTTU, generated by Polson (2008) and used by Du Toit (2008), were investigated.

5.2.3.1 Outlet region

All the spheres, whose centre coordinates fell within a region of $0.3 \text{ m} \leq r \leq 0.63 \text{ m}$ and $1.05 \text{ m} \leq z \leq 1.17 \text{ m}$, were extracted from the numerically generated annular packed bed of Polson (2008). The centre coordinates of these spheres were then inserted into SolidWorks® to generate a virtual representation of the packing. Next the free flow volume around the spheres was extracted for a region defined as $0.3 \text{ m} \leq r \leq 0.6 \text{ m}$ and $1.08 \text{ m} \leq z \leq 1.2 \text{ m}$. The free flow region was then cut into smaller annular rings with an annular width and a height of 10 mm. This procedure resulted in 360 smaller annular rings for which the free flow volume was determined using SolidWorks®'s mass properties application. Since both the free flow and total volume of each

annular ring were known the average porosity of each annular ring could be determined. This yielded the average porosity distribution for the outlet region of the packed bed.

5.2.3.2 Two-wall inlet region

For the two-wall inlet region the same approach was followed as for the outlet region. All the spheres, whose centre coordinates fell within a region of $0.3 \text{ m} \leq r \leq 0.63 \text{ m}$ and $0 \text{ m} \leq z \leq 0.33 \text{ m}$, were extracted from Polson's (2008) numerically packed bed. A virtual representation of the packing was once again created in SolidWorks®, using the centre coordinates of the removed spheres, from which the free flow region, confined to $0.3 \text{ m} \leq r \leq 0.6 \text{ m}$ and $0 \text{ m} \leq z \leq 0.3 \text{ m}$, was extracted. The free flow region was once again cut into smaller annular rings with an annular width and height of 10 mm and the average porosity for each annular ring was accordingly determined. This procedure once again yielded the average porosity distribution for the packing in the inlet region of the bed where two walls disturb the packing structure.

5.2.4 Results and discussion

To investigate the modelling methodology, the axial ($\varepsilon(z)$) and radial ($\varepsilon(r)$) variations in porosity were predicted using equation (2.6). These porosity values were then combined using equations (5.1) and (5.2) to predict the porosity distribution in the outlet and inlet regions of the bed. A comparison between the predicted and numerically measured porosity distributions, for the in and outlet region of the bed, is shown in Figure 5-3 and Figure 5-4.

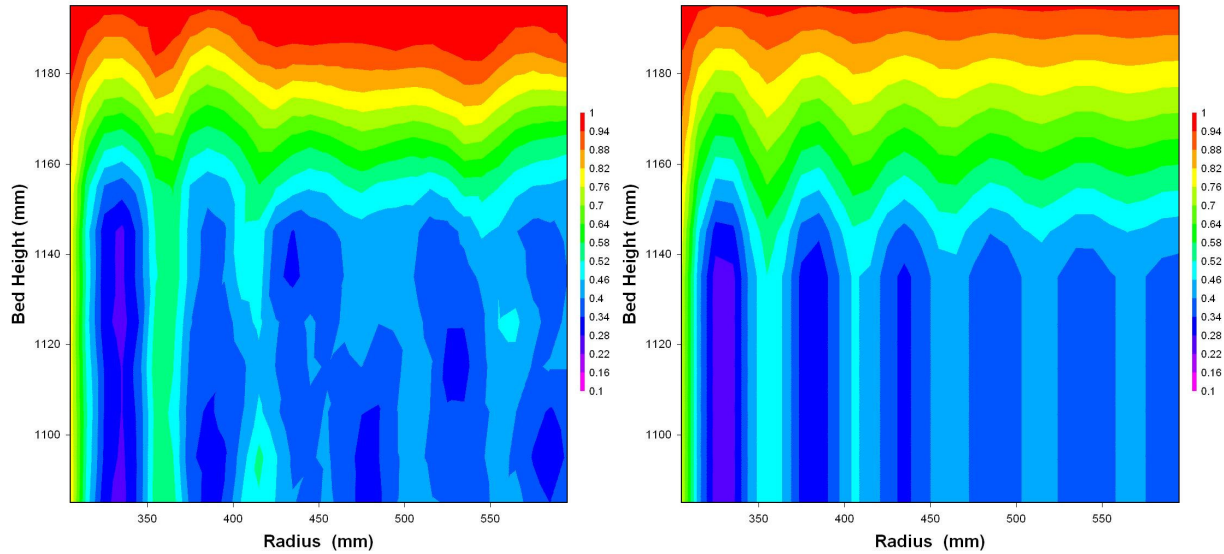


Figure 5-3: Comparison between the numerically measured (left) and predicted (right) porosity distribution in the outlet region of the packed bed.

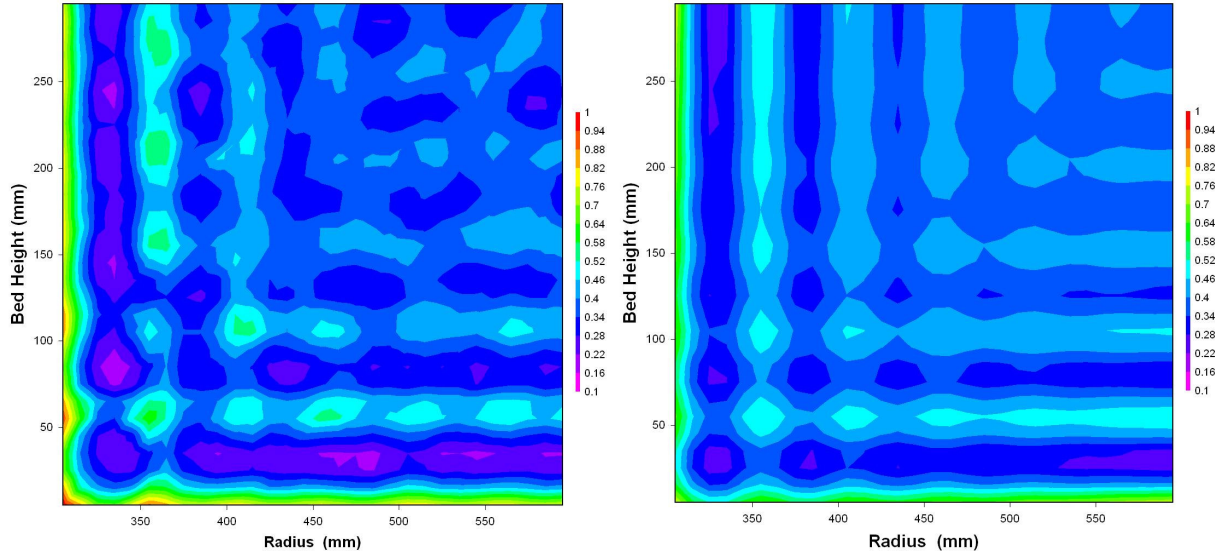


Figure 5-4: Comparison between the numerically measured (left) and predicted (right) porosity distribution in the inlet region of the bed where two walls disturb the packing structure.

From Figure 5-3 it can be seen that equation (5.1) predicts a porosity distribution that is very similar to the porosity distribution obtained from the numerically packed bed. In the numerically packed bed the outlet of the bed is set at a distance of 30 mm from the centre of the highest sphere in the packing. Due to the randomness of the packing, a lot of spheres may be positioned near the defined bed outlet but these spheres will however be positioned lower than the sphere, used to define the outlet. This phenomenon is not accounted for by the correlations used to describe the structure of the bed. This explains why a larger region of higher porosity, near the outlet of the bed at $L=1.2$ m, is observed for the numerically packed bed and why this region of high porosity is not present in the predicted porosity distribution. It should be remembered that the porosity distribution correlations are unable to predict the actual structure of the bed and are only approximations that predict the average structure of the bed. In Figure 5-4 it can be seen that equation (5.2) yields a porosity distribution that is very similar to the porosity distribution of the numerically packed bed.

It can be concluded that equations (5.1) and (5.2) can be used to represent the structure of the packed bed in the bed's outlet region and inlet region where the packing is disturbed by the two walls.

5.3 Fluid Flow through the HTTU's packed bed (FF Cases)

5.3.1 Description

Du Toit (2008) found the damped oscillatory porosity correlation of Martin (1978) to be superior in describing the structure of the annular packed bed of the HTTF. His investigation did however not include the porosity correlation proposed by De Klerk (2003). The correlation of De Klerk (2003) seemed superior to the correlation of Martin (1978) when compared with the porosity distribution of the HTTF, presented by Du Toit (2008).

The FF case simulations were conducted in order to investigate the influence each correlation had on the fluid distribution and which correlation yielded a fluid distribution similar to that which had been obtained experimentally. The FF case simulations were also conducted in order to verify the simulation methodology to be used in the explicit modelling of a packed bed.

Case FF-1 employed the porosity correlation of De Klerk (2003), while case FF-2 employed the correlation proposed by Martin (1978).

The geometry used in the numerical analysis of the FF cases consisted of a 1/32 axis-symmetrical cut of the HTTU's geometry. Regions of complex geometry (heater and outer annulus wall) were replaced with simplified geometries. The final geometry used in the FF cases is shown in Figure 5-5 while the values of the geometric parameters are given in Table 5-1.

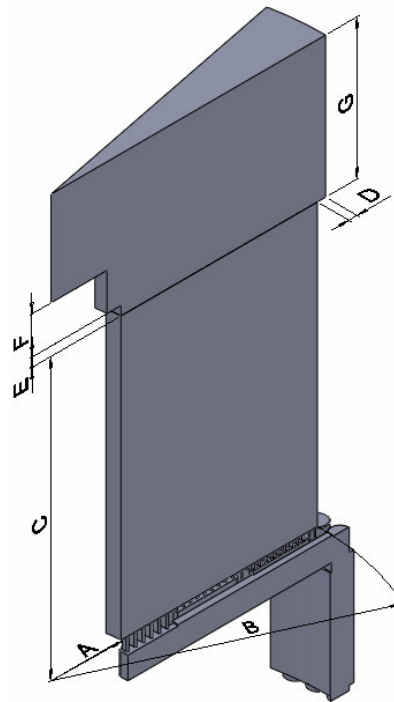


Figure 5-5: FF case geometry

Table 5-1: Geometric parameters of FF case

Parameter	Description	Value
A	Inner annulus radius (R_i)	300.00 mm
B	Outer annulus radius (R_o)	1143.07 mm
C	Bed length (L)	1200.00 mm
D	Distance from outer annulus wall to confining wall	35.33 mm
E	Protrusion length of heater casing above bed outlet	38.10 mm
F	Protrusion length of heater elements above heater casing	160.00 mm
G	Distance from top of bed to outlet	600.00 mm

5.3.2 Computational domain, physics models and boundary conditions

In order to investigate the influence the different damped oscillatory porosity correlations had on the fluid distribution through an implicitly modelled packed bed, the fluid domain was created as shown in Figure 5-5. The bed was assumed to be axi-symmetrical around the axis of the annulus. These FF cases also served to verify the implicit bed modelling methodology. Nitrogen, at a temperature of 20.1 °C and a pressure of 100.15 kPa , was used as the fluid. The simulation model was set-up and solved in the commercial RANS CFD code, STAR-CCM+®.

The computational domain contained three individual regions as shown in Figure 5-6. The outlet and header inlet regions were modelled as fluid regions while the packed bed was modelled as a porous region. To ensure fluid flow occurred between the different regions, interfaces were created on the contacting surfaces between the individual regions.

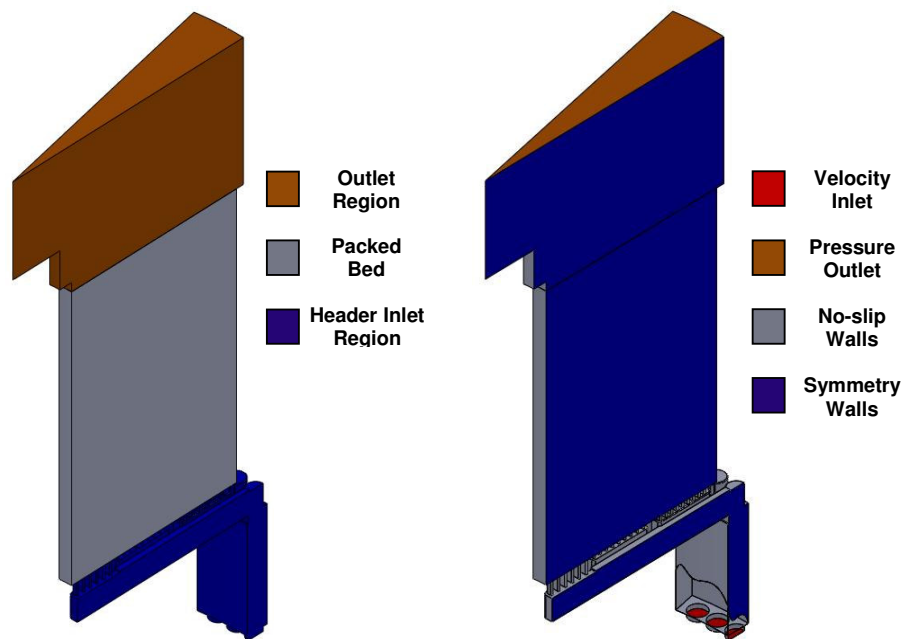


Figure 5-6: Regions (left) and boundary types (right) of the FF case computational domain.

The boundary types used in the FF case simulations included velocity inlets, pressure outlets, no-slip walls and symmetry walls. The type and location of boundaries used can be seen on the right in Figure 5-6. For the velocity inlet a uniform velocity of 1.08 m/s was specified. This corresponds to a mass flow of 0.5 kg/s and a superficial velocity (V_0) of 0.1136 m/s through the annulus. The relative pressure of the pressure outlet was set to 0 Pa. This pressure was relative to a pressure of 100.15 kPa. For both the in - and outlet a turbulence intensity of 5% and fluid temperature of 20.1 °C was specified.

The computational mesh was generated using the built-in meshing tool of STAR-CCM+®. The computational mesh consisted of a mixed structured and unstructured mesh. The structured mesh was generated adjacent to the no-slip walls, shown in Figure 5-6, while the rest of the mesh was unstructured and consisted of polyhedral cells. The structured mesh consisted of five layers of prismatic cells (prism layers). The total prism layer thickness was confined to 5mm while the thickness of each individual layer was scaled by a ratio of 1.5. In the generation of the surface mesh a maximum and minimum surface size of 6.0 and 1.0 mm was chosen. The surface growth rate was set to 1.3.

In the simulation the $k-\varepsilon$ turbulence model was used. For the wall treatment, the two-layer wall treatment model with the realizable $k-\varepsilon$ turbulence model was used. The fluid flow was assumed to be three dimensional, stationary and steady. Nitrogen was assumed to be an isothermal ideal gas.

Measurements of velocity were taken at a distance of 60 mm from the bed exit. These velocity measurements were compared with the adjusted velocity profile, as described in chapter 4.4, so as to verify the modelling methodology used.

The simulations were presumed as converged once the residuals have reached a steady value. The mass flow and pressures on the interfaces, between the individual regions, were also used as additional convergence monitors. These were also presumed as converged once they reached a steady value.

5.3.3 Mathematical formulation

Since the spheres and pores are modelled implicitly, a porosity correlation was used to describe the structure of the packed bed. For FF-1 the correlation of De Klerk (2003) was used and for FF-2 the correlation of Martin (1978) was used. These correlations were derived for a cylindrical packed bed. It was assumed that the porosity distribution was symmetrical about the centre of the annular region ($[R_o + R_i]/2$). These correlations can also be used to predict the axial variation in porosity if they are made to be dependent on the axial distance away from the bed support wall rather than the radial distance away from the container wall.

For FF-1 the radial and axial variation in porosity was written as:

$$\varepsilon(r) = \begin{cases} 2.14x^2 - 2.53x + 1 & \text{for } x \leq 0.637 \\ \varepsilon_b + 0.29e^{-0.6x} \cos(2.3\pi(x - 0.16)) + 0.15e^{-0.9x} & \text{for } x > 0.637 \end{cases} \quad (5.3)$$

with

$$x = \begin{cases} \frac{r - R_i}{d_p} & \text{for } R_i \leq r \leq \frac{R_o + R_i}{2} \\ \frac{R_o - r}{d_p} & \text{for } \frac{R_o + R_i}{2} \leq r \leq R_o \end{cases} \quad (5.4)$$

and

$$\varepsilon(z) = \begin{cases} 2.14y^2 - 2.53y + 1 & \text{for } y \leq 0.637 \\ \varepsilon_b + 0.29e^{-0.6y} \cos(2.3\pi(y - 0.16)) + 0.15e^{-0.9y} & \text{for } y > 0.637 \end{cases} \quad (5.5)$$

with

$$y = \frac{z - z_0}{d_p} \quad \text{for } z \geq z_0 \quad (5.6)$$

where y is the dimensionless distance from the bed support wall, z_0 the axial coordinate of the bed support wall and z the axial coordinate.

For FF-2 the radial and axial variation in porosity was written as:

$$\varepsilon(r) = \begin{cases} \varepsilon_{\min} + (1 - \varepsilon_{\min})x^2 & \text{for } -1 \leq x \leq 0 \\ \varepsilon_b + (\varepsilon_{\min} - \varepsilon_b)e^{\frac{-x}{4}} \cos\left(\frac{\pi}{C}x\right) & \text{for } x \geq 0 \end{cases} \quad (5.7)$$

with

$$x = \begin{cases} 2\frac{r - R_i}{d_p} - 1 & \text{for } R_i \leq r \leq \frac{R_o + R_i}{2} \\ 2\frac{R_o - r}{d_p} - 1 & \text{for } \frac{R_o + R_i}{2} \leq r \leq R_o \end{cases} \quad (5.8)$$

and

$$\varepsilon(z) = \begin{cases} \varepsilon_{\min} + (1 - \varepsilon_{\min})y^2 & \text{for } -1 \leq y \leq 0 \\ \varepsilon_b + (\varepsilon_{\min} - \varepsilon_b)e^{\frac{-y}{4}} \cos\left(\frac{\pi}{C}y\right) & \text{for } y \geq 0 \end{cases} \quad (5.9)$$

with

$$y = 2\frac{z - z_0}{d_p} - 1 \quad \text{for } z \geq z_0 \quad (5.10)$$

In both cases (FF-1 & FF-2) the bulk porosity was taken as $\varepsilon_b = 0.39$ and the minimum porosity was taken as $\varepsilon_{\min} = 0.23$ in FF-2.

In order to define the porosity distribution throughout the entire annular bed, the bed was divided into six regions as shown in Figure 5-7.

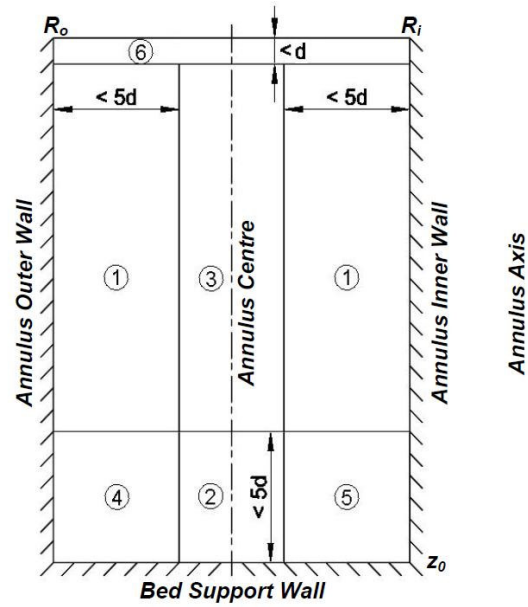


Figure 5-7: Different porous regions in annular packed bed

Table 5-2 summarises the equations used to define the porosity of each region in the bed. Figure 5-8 shows the obtained porosity distribution of the packed bed for FF-2.

Table 5-2: Summary of equations used to describe the beds porosity distribution

Region	Equations Describing Region's Structure	
	FF-1	FF-2
1	(5.3) with (5.4)	(5.7) with (5.8)
2	(5.5) with (5.6)	(5.9) with (5.10)
3	Average of (5.3) & (5.5)	Average of (5.7) & (5.9)
4	(5.2) with (5.3) & (5.5)	(5.2) with (5.7) & (5.9)
5	(5.2) with (5.3) & (5.5)	(5.2) with (5.7) & (5.9)
6	(5.1) with (5.3)	(5.1) with (5.7)

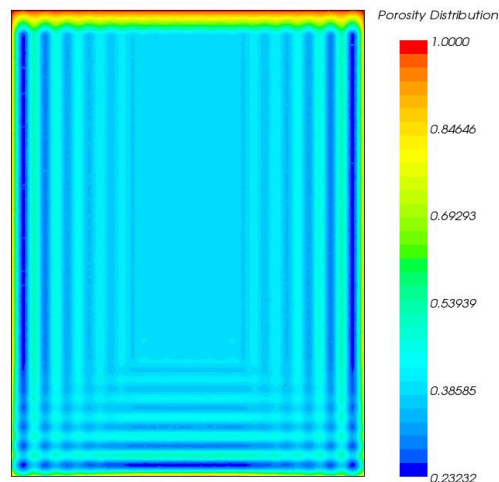


Figure 5-8: Representation of porosity distribution through the packed bed for FF-2.

In STAR-CCM+® the resistance of the porous medium is modelled through the insertion of a porous source term into the momentum equations. This source term is defined as:

$$\mathbf{f}_p = R \cdot \vec{V}_0 \quad (5.11)$$

where $\mathbf{f}_p$ constitutes the porous source term, R is the porous resistance tensor and $\vec{V}_0 = \vec{V}_0(r, \theta, z) = (V_{0r}(r, \theta, z); V_{0\theta}(r, \theta, z); V_{0z}(r, \theta, z))$ the superficial velocity through the porous medium. The porous resistance tensor is in turn defined as:

$$R = R_v + R_i \cdot |\vec{V}_0| \quad (5.12)$$

where R_v and R_i are the viscous and inertial resistance tensors respectively. Using the KTA (1981) pressure drop correlation, as presented in equation (2.18), the viscous and inertial porous resistance tensors were defined as:

$$R_v = \begin{Bmatrix} R_{vr} & 0 & 0 \\ 0 & R_{v\theta} & 0 \\ 0 & 0 & R_{vz} \end{Bmatrix} \quad (5.13)$$

with

$$R_{vr} = R_{v\theta} = R_{vz} = 160 \frac{(1 - \varepsilon(r, z))^2}{\varepsilon(r, z)^3} \frac{\mu_f}{d_p^2} \quad (5.14)$$

where R_{vr} constitutes the radial viscous porous resistance, $R_{v\theta}$ the tangential viscous porous resistance and R_{vz} the axial viscous porous resistance, and

$$R_i = \begin{Bmatrix} R_{ir} & 0 & 0 \\ 0 & R_{i\theta} & 0 \\ 0 & 0 & R_{iz} \end{Bmatrix} \quad (5.15)$$

with

$$\begin{aligned} R_{ir} &= 3 \frac{(1 - \varepsilon(r, z))^{1.1}}{\varepsilon(r, z)^3} \left(\frac{\mu_f}{\rho |V_{0r}(r, \theta, z)| d_p} \right)^{0.1} \frac{\rho}{d_p} \\ R_{i\theta} &= 3 \frac{(1 - \varepsilon(r, z))^{1.1}}{\varepsilon(r, z)^3} \left(\frac{\mu_f}{\rho |V_{0\theta}(r, \theta, z)| d_p} \right)^{0.1} \frac{\rho}{d_p} \\ R_{iz} &= 3 \frac{(1 - \varepsilon(r, z))^{1.1}}{\varepsilon(r, z)^3} \left(\frac{\mu_f}{\rho |V_{0z}(r, \theta, z)| d_p} \right)^{0.1} \frac{\rho}{d_p} \end{aligned} \quad (5.16)$$

where R_{ir} constitutes the radial inertial porous resistance, $R_{i\theta}$ the tangential inertial porous resistance, R_{iz} the axial inertial porous resistance and $\varepsilon(r, z)$ was determined as described in Table 5-2.

Since equation (5.16) contains a velocity term below the line, regions of stagnant fluid flow would yield undefined inertial porous resistance values. To avoid this from occurring, a logical test was built into the equation. In the test, the superficial velocity components were evaluated for stagnant flow. If the velocity component was found to have a magnitude less than 1×10^{-7} m/s, a velocity magnitude of 1×10^{-7} was assigned to the velocity component before the porous resistance values, as per equation (5.16), were determined. A representation of the inertial and viscous resistance distributions can be seen in Figure 5-9.

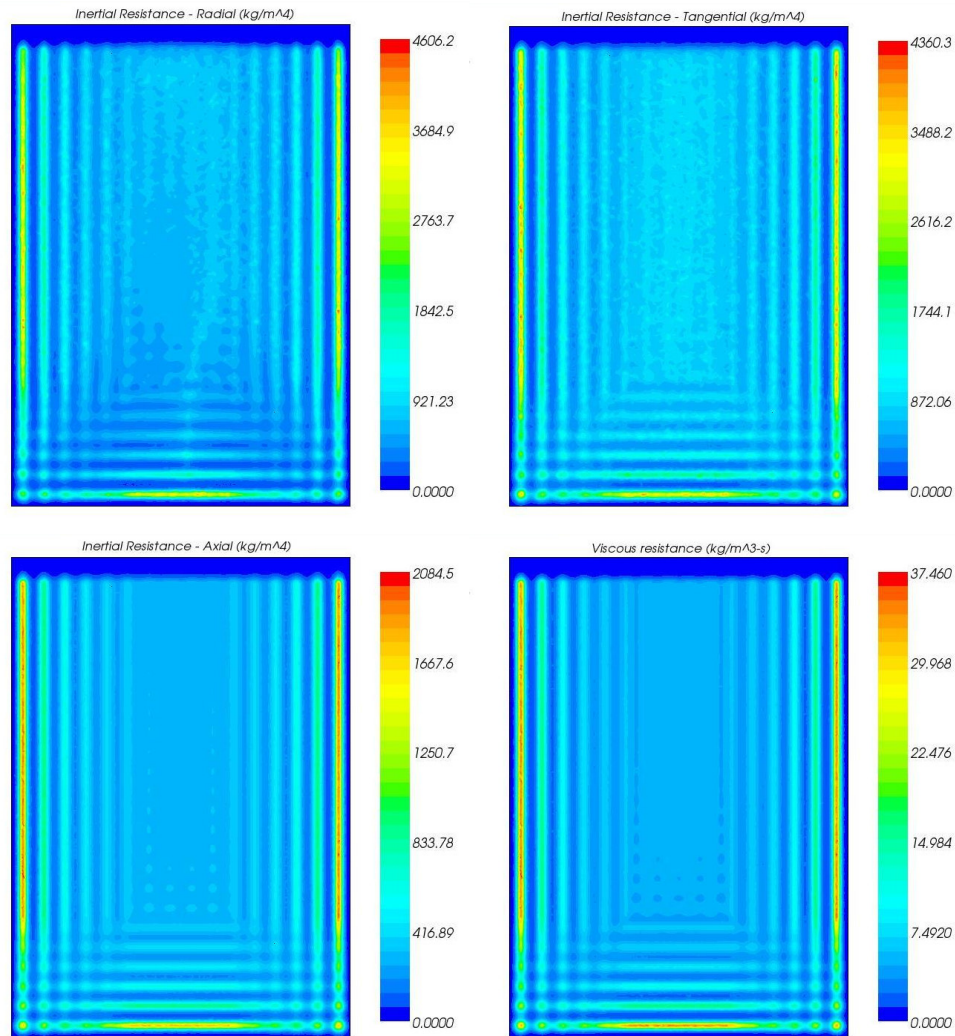


Figure 5-9: Representation of porous resistance distributions for FF-2 (top left: R_{ir} , top right: $R_{i\theta}$, bottom left: R_{iz} & bottom right: R_v)

The effective viscosity model, proposed by Giese *et al.* (1998), was used to model the fluid flow in the near wall region. This model is represented in equation (2.21). The dynamic viscosity, in the RANS equations, was replaced with the effective viscosity, while the dynamic viscosity was employed to calculate the viscous and inertial porous resistance terms.

5.3.4 Results and discussion

A comparison between the predicted velocity profiles for each FF case and the modified experimental velocity profile is shown in Figure 5-10. The predicted profiles were obtained 60 mm from the exit of the bed.

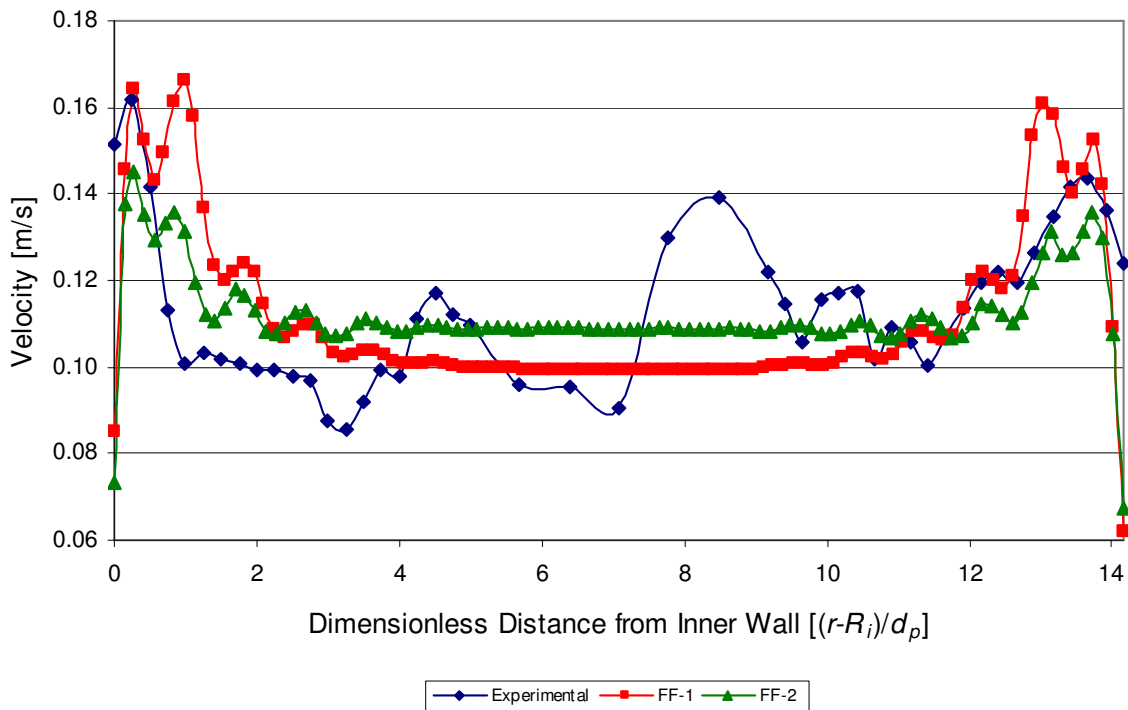


Figure 5-10: Comparison velocity profiles predicted by the FF cases and the measured profile

The velocity peaks, adjacent to the annulus wall, is predicted fairly accurately in FF-1. The magnitude of the second velocity peak is however over predicted. In FF-2 the position of the velocity peaks are predicted correctly. The magnitude of these velocity peaks is however under predicted. This indicates that the effective viscosity value is too large. A second velocity peak is also predicted by FF-2. The magnitude of this second peak is significantly lower than the peak predicted by FF-1. This is because the porosity correlation, used in FF-1, predicts a higher second peak in porosity than the correlation used in FF-2. This variation in porosity can be seen in Figure 2-6. The porous resistance, in this region of higher porosity, is thus significantly lower and would allow more fluid to flow through this region, explaining the over prediction of the second velocity peak in FF-1.

In order to establish which test case predicted the velocity profile better, the percentage deviation between the measured and predicted velocity profiles were calculated using the L2 or Euclidean error norm. This error norm is defined as:

$$\% \text{ Deviation} = \sqrt{\frac{\sum_{i=1}^n (V_{si} - V_{mi})^2}{\sum_{i=1}^n (V_{mi}^2)}} \times 100 \quad (5.17)$$

where V_{si} and V_{mi} is the average simulated and measured velocity over the small annular rings.

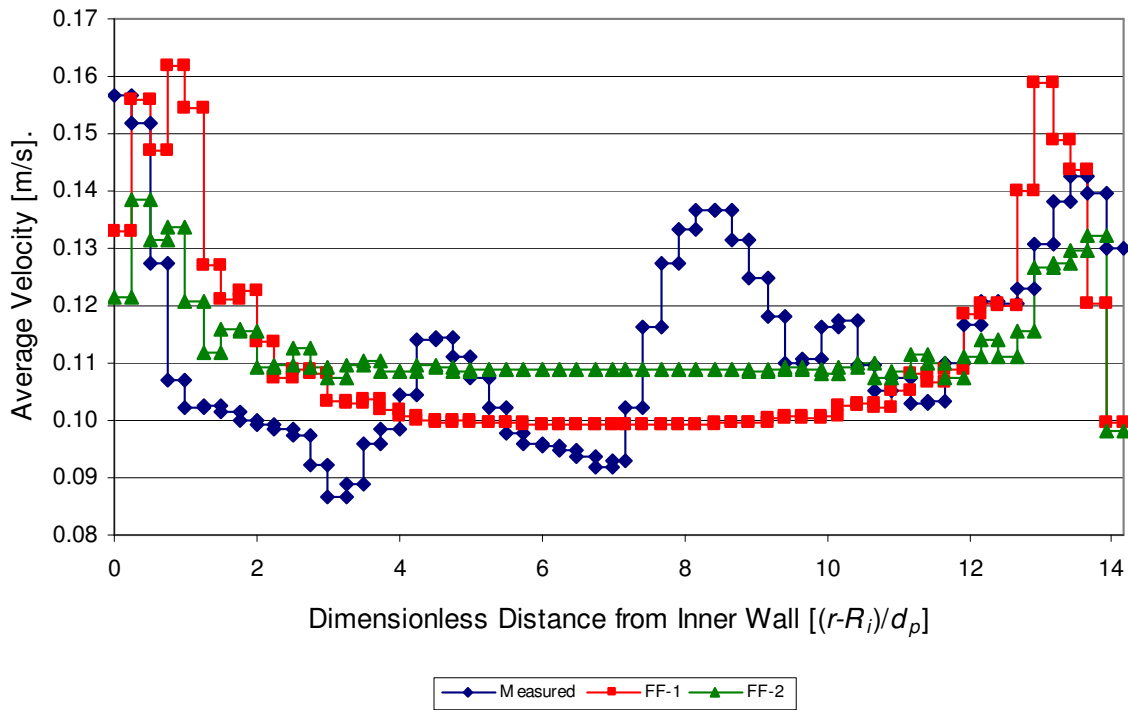


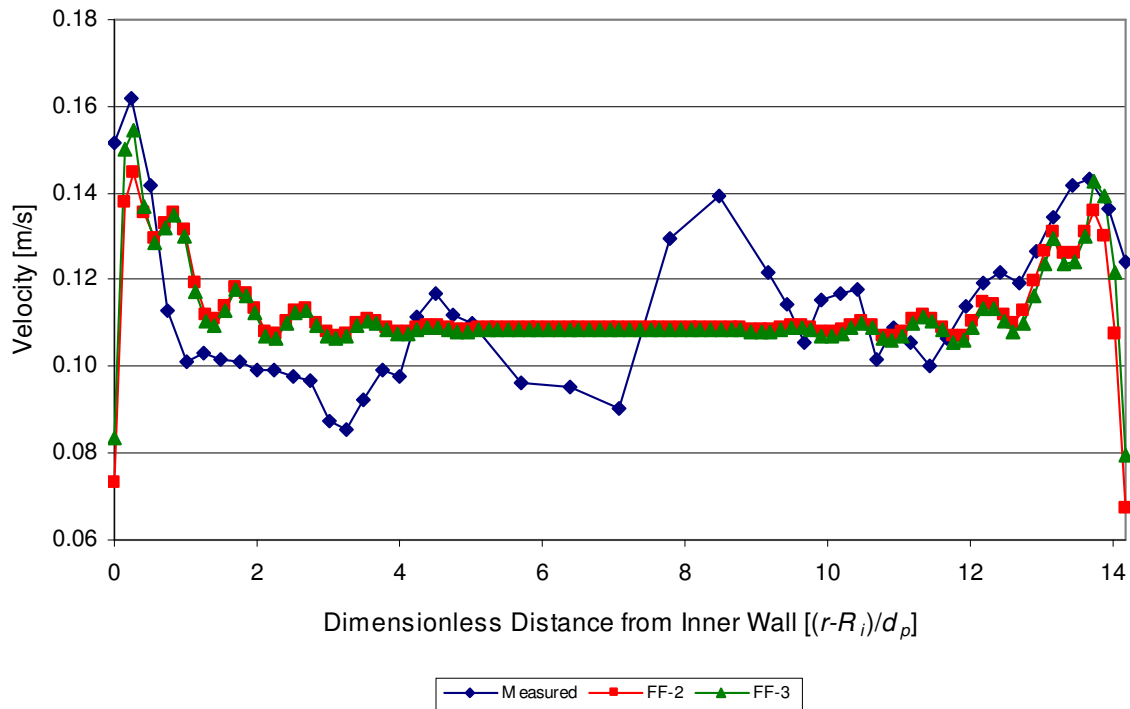
Figure 5-11: Average Velocity profiles, calculated for an annular width of $\frac{1}{4} d_p$

These average velocities were determined by dividing the velocity profile into a number of smaller annular rings with a predetermined annular width. The volume flow rate through each annular ring was calculated by integrating the velocity profile over the particular annular ring. The average velocity for the annular ring was then calculated by dividing the calculated mass flow rate by the free flow area of the annular ring. This was done for annular widths of $\frac{1}{4} d_p$, $\frac{1}{2} d_p$, $\frac{3}{4} d_p$ and $1 d_p$. A comparison between the average velocities, calculated for an annular width of $\frac{1}{4} d_p$, is shown in Figure 5-11 while the percentage deviation for different annular ring widths is shown in Table 5-3.

Table 5-3: Percentage deviation of FF case velocity profiles from measured velocity profile

<i>Annular Width</i>	<i>% Deviation</i>	
	<i>FF-1</i>	<i>FF-2</i>
$1/4 d_p$	16.70%	12.69%
$1/2 d_p$	15.85%	12.12%
$3/4 d_p$	15.42%	11.53%
$1 d_p$	13.60%	10.83%

From Table 5-3 it can be seen that the velocity profile, predicted by the simulation case FF-2, is a closer fit to the measured velocity profile than the profile obtained in case FF-1. The magnitude of the velocity peaks, predicted in case FF-2, is however lower than the velocity peaks of the measured velocity profile. For this reason the value of the effective viscosity was reduced by a factor of 0.8. This simulation case was designated as FF-3. The result of the reduction in effective viscosity can be seen in Figure 5-12.

**Figure 5-12: Influence of effective viscosity on predicted velocity distribution**

From Figure 5-12 it can be seen that the use of a smaller effective viscosity had the largest effect on the velocity peak magnitudes in the near wall region. The percentage deviation between the measured and predicted velocity distributions are shown in Table 5-4.

Table 5-4: Influence of effective viscosity on percentage deviation between measured and simulated velocity profiles

Annular Width	% Deviation	
	FF-2	FF-3
$1/4 d_p$	12.69%	11.84%
$1/2 d_p$	12.12%	11.38%
$3/4 d_p$	11.53%	10.93%
$1 d_p$	10.83%	10.43%

It is clear that the reduction in effective viscosity yielded a velocity profile that is a better fit to the measured profile. Further reduction of the effective viscosity would further increase the magnitude of the velocity peaks adjacent to the annulus walls but could increase the percentage deviation between the simulated and measured velocity profiles.

Due to the dependence of the near wall velocity region on the effective viscosity it may be argued that an effective viscosity, which is dependant on the structure of the bed, will be more suited in the modelling approach than a constant effective viscosity. A few attempts, at employing a porosity dependant effective viscosity, were carried out. One such attempt was to modify the effective viscosity correlation of Giese et al. (1998) as follows:

$$\frac{\mu_{eff}}{\mu_f} = 2 \exp(3.5 \times 10^{-3} \text{Re}) \frac{\epsilon_b}{\epsilon(r, z)} \quad (5.18)$$

These attempts did not yield any improvement in the predicted velocity profile. The measured velocity profiles offer no insight into the velocity distribution inside the packed bed. For this reason it was impossible to derive a structure dependant effective viscosity and it was deemed to be beyond the scope of this study to derive such a correlation. The need for a structure dependant effective viscosity model still remains as it not only influences the velocity profile but also the pressure drop through the packed bed.

Figure 5-13 shows how the velocity distribution of FF-3 compares with the normalised average experimental velocity profiles. These profiles are the average profiles calculated from three velocity tests, per mass flow rate. They were normalised as follows:

$$\frac{V_i}{V_{0calc}} = \frac{V_i}{\frac{\int_{R_i}^{R_o} \int_0^{2\pi} V_i(r) dr d\theta}{2\pi(R_o^2 - R_i^2)}} \quad (5.19)$$

In chapter 4 it was found that the axial velocity profile can be extracted from the experimental velocity profile using a factor of 0.801. The factor was determined for a mass flow rate of 0.5 kg/s and could differ for other

mass flow rates. In order to circumvent the need to explicitly model the bed for each mass flow rate, the profiles were normalised using equation (5.19). This equation uses a numerically calculated superficial velocity instead of the superficial velocity calculated from the mass flow rate ($V_o = m / \rho A$). This calculated superficial velocity was obtained by dividing the numerically calculated volume flow rate (obtained by the integration of the velocity profile over the entire annular region) by the free flow area of the annulus. By normalizing the profiles in this manner, the error in measurement, due to measuring the resultant of the axial and radial velocity components, is eliminated.

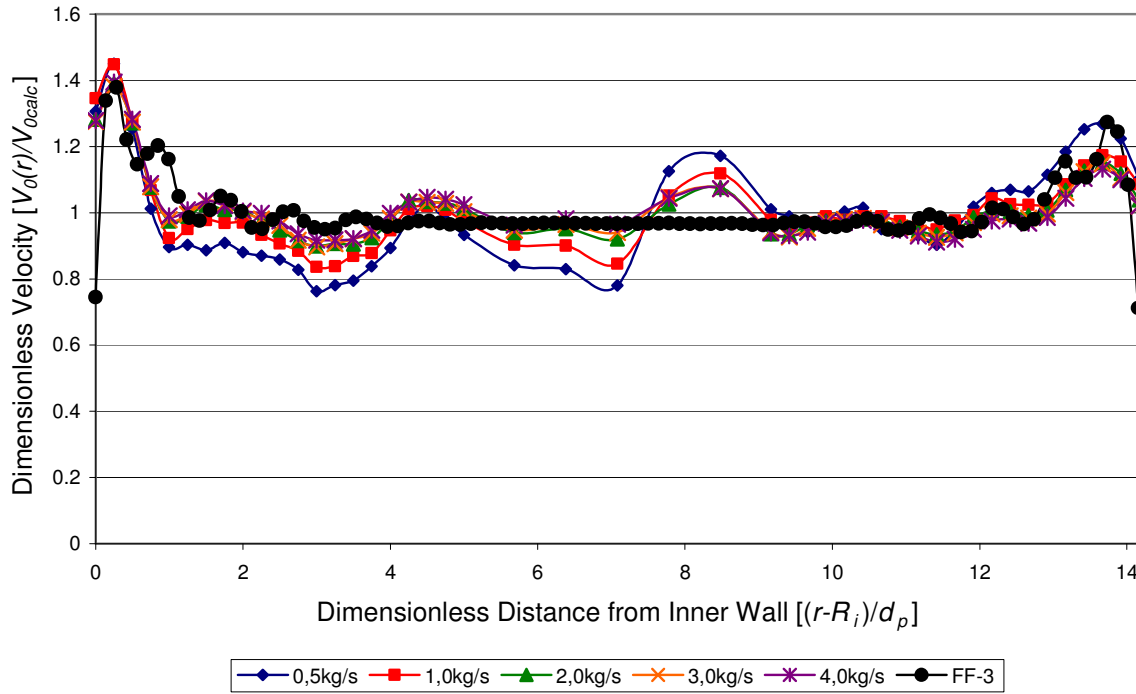


Figure 5-13: Normalized velocity distribution (measured vs. predicted)

Even though the velocity profile of FF-3 was obtained for a mass flow rate of 0.5kg/s it shows better agreement with the velocity profiles obtained for higher mass flow rates. It should be remembered that the model is based on an empirical correlation describing the structure of the bed. It is however impossible to predict the actual structure of the bed used during the experiments. Because of this, certain deviations will occur between the measured and simulated velocity profiles. The simulated velocity profile shows fair agreement with the measured velocity profiles and further adjustments to the simulation model would not yield any more improvements.

Based on this, it was decided that the methodology used in case FF-3 was the best suited for the investigation of the fluid distribution through an annular packed bed. This study is described in the next section.

5.4 Velocity distribution through an annular packed bed (VD Case)

5.4.1 Description

The velocity distribution (VD) case was conducted to investigate the development of the fluid flow distribution through an annular bed, consisting of randomly packed spheres. Using the methodology of simulation case FF-3, as discussed in section 5.3.4, the bed was modelled as a porous medium in which the presence of the pores and spheres were accounted for implicitly. The simulation was once again set-up in the commercial RANS CFD code STAR-CCM+®. The geometry used in the simulation model is shown in Figure 5-14 while the values and description of the geometric parameters are given in Table 5-5.

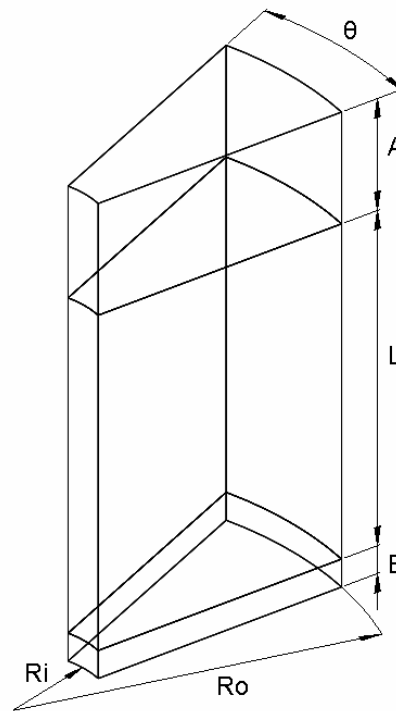


Figure 5-14: VD case geometry

Table 5-5: Geometric parameters of VD case

Parameter	Description	Value
R_i	Inner annular radius	300 mm
R_o	Outer annular radius	1150 mm
θ	Pie segments of annular bed	24 °
A	Outlet length	500 mm
B	Inlet length	100 mm
L	Packed bed height	1200 mm

5.4.2 Computational domain, physics models and boundary conditions

As with the FF case simulations in chapter 5.3, the computational domain of the VD case simulation contained three independent regions. These regions are shown on the left of Figure 5-15. In the model the in- and outlet regions were modelled as fluid regions while the packed bed was modelled as a porous medium. The fluid was taken to be nitrogen at a temperature and pressure of 20.1 °C and 100.15 kPa. To allow flow interaction between the regions, interfaces were created between the touching surfaces of the regions. These interfaces, along with all the boundary types, used in the model, are shown on the right of Figure 5-15.

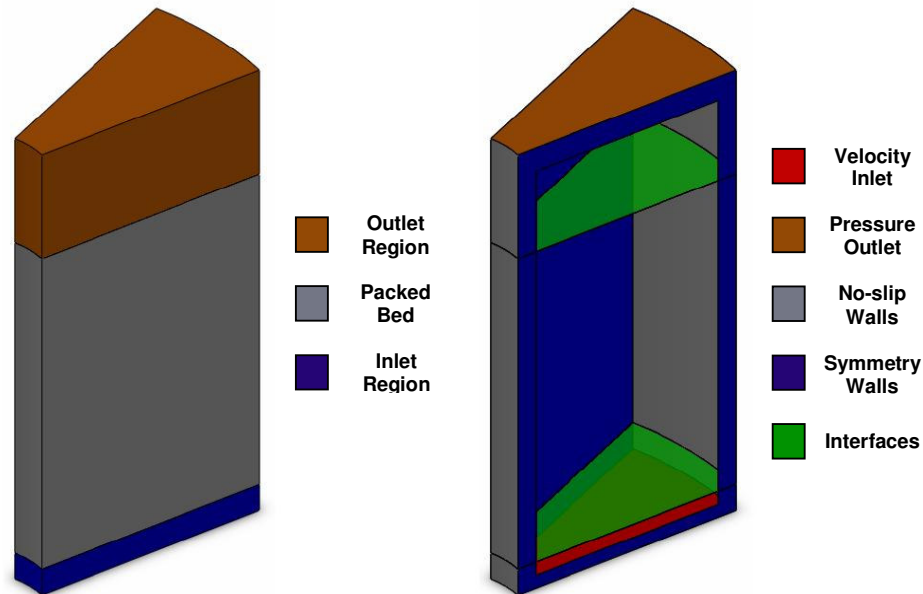


Figure 5-15: VD case regions (left) and boundary types (right)

At the velocity inlet a uniform velocity (V_0) of 0.1122 m/s was specified. This corresponded to a mass flow rate of 0.50 kg/s through the annulus and a Reynolds number of $Re = 432$. The temperature of the nitrogen entering the fluid domain was set at 20.1 °C. At the pressure outlet boundary a relative pressure of 0 kPa was specified. This pressure is relative to the reference pressure of 100.15 kPa. Turbulent flow was modelled through the use of the $k - \varepsilon$ turbulence model. The turbulence intensity of the fluid entering and exiting the computational domain was specified as 5%.

The computational mesh was once again generated using the built-in meshing tool of STAR-CCM+®. The mesh was a mixed structured and unstructured mesh. The structured mesh was generated adjacent to the no-slip wall and consisted of 5 prismatic cell layers. These layers were scaled by a ratio of 1.5 and had a total thickness of 5 mm. The unstructured mesh consisted of polyhedral cells. During the generation of the surface mesh a minimum and maximum surface size of 1 and 6 mm was specified respectively. A surface growth rate of 1.3 was used.

The mathematical formulation of the porous region was the same as that of simulation case FF-3 in section 5.3.3. The velocity in the near-wall region was modelled using the effective viscosity of Giese *et al.* (1998). From the fluid flow cases of section 5.3 it was found that adjusting the effective viscosity by a factor of 0.8 yielded velocity profiles that showed fair agreement with the measured profiles. For this reason the effective viscosity was adjusted by a factor of 0.8.

The fluid flow was assumed to be three-dimensional and steady while the model is stationary. The simulation was judged to be converged once the residuals reached a steady value. The mass flow rate through the interfaces, shown in Figure 5-15, along with the pressure drop over the porous region were monitored and used as additional convergence measures.

In order to establish the development of the velocity profile through the bed, the velocity was measured at height intervals of 1 particle diameter (60 mm) starting 60 mm from the bed support wall. To obtain a good indication of the velocity profile, at a certain height inside the bed, five line probes were used to numerically measure the velocity. Each line probe contained 251 measuring points that were equally spaced out over the width of the annulus. The average velocity profile for each height was then calculated from velocity profiles obtained from the five line probes. The different heights at which measurements were taken along with the position of the five line probes, on the plane of measurement, are shown in Figure 5-16.

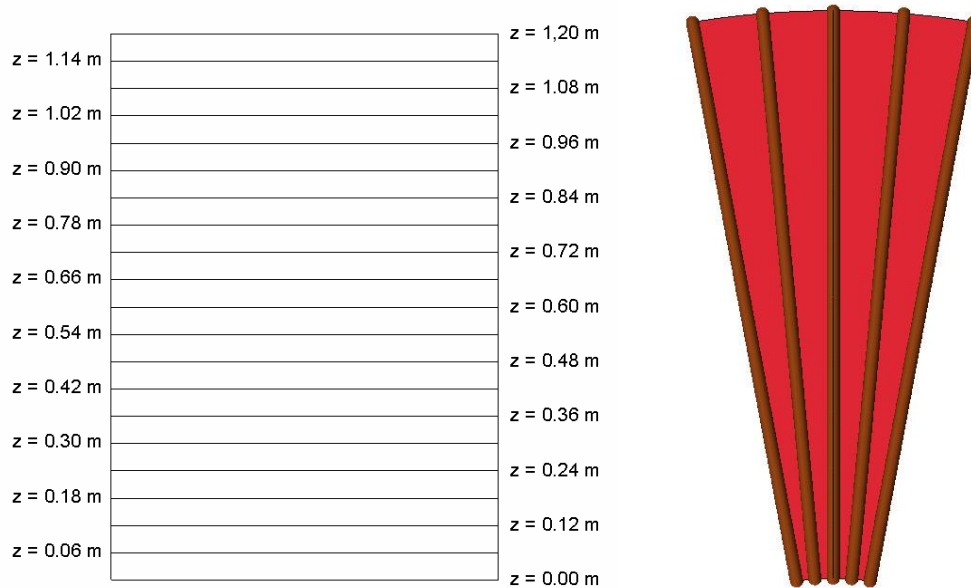


Figure 5-16: Velocity measurement heights (lefts) and measurement probes (right)

5.4.3 Results and discussion

The normalised velocity distribution profiles for the inlet, bulk and outlet region are shown in Figure 5-17, Figure 5-18 and Figure 5-19.

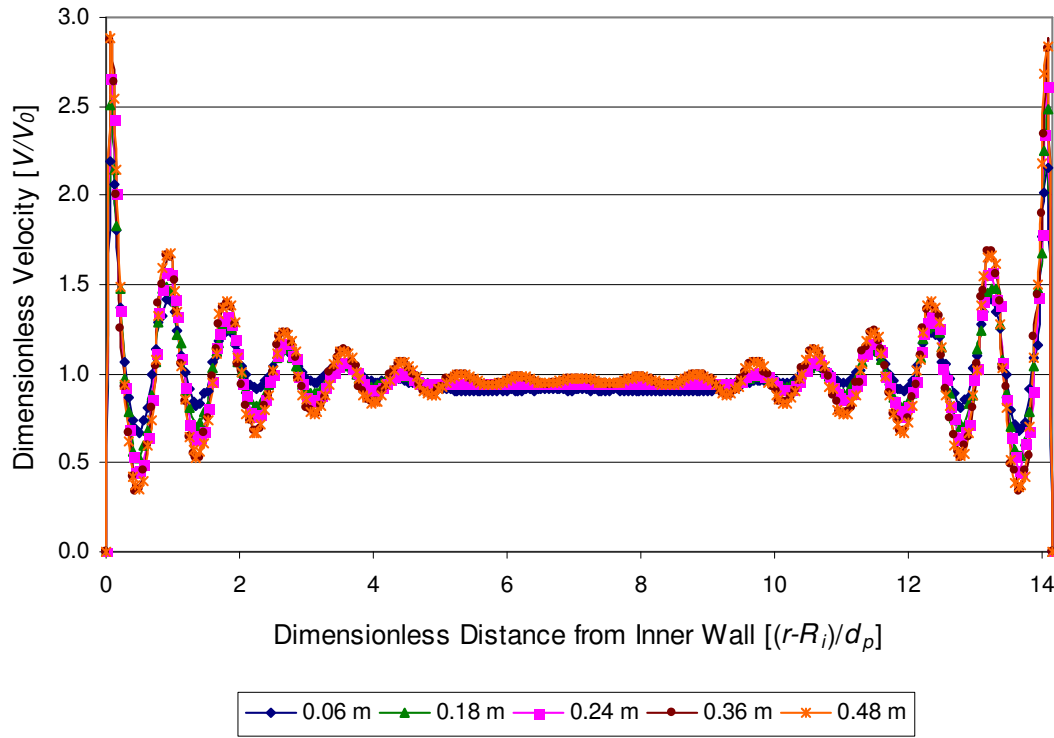


Figure 5-17: Velocity distribution through bed's inlet region

From Figure 5-17 it can be seen that the basic shape of the velocity profile is already established within a distance of one particle diameter from the bed support wall. The amplitude of the velocity peaks are however smaller than the velocity peaks of the fully developed velocity profile. The magnitude of these peaks increases gradually as fluid is channelled from the regions of lower porosity to regions of higher porosity. The dependence of the fluid flow distribution on the bed's structure/porosity is also clearly visible. The velocity profile is still developing in the inlet region of the bed due to the unsettled structure of the packing. The fluid flow only becomes fully developed once the structure of the bed has settled ($0.3 \text{ m} \leq z \leq 1.14 \text{ m}$). This can be seen in Figure 5-18.

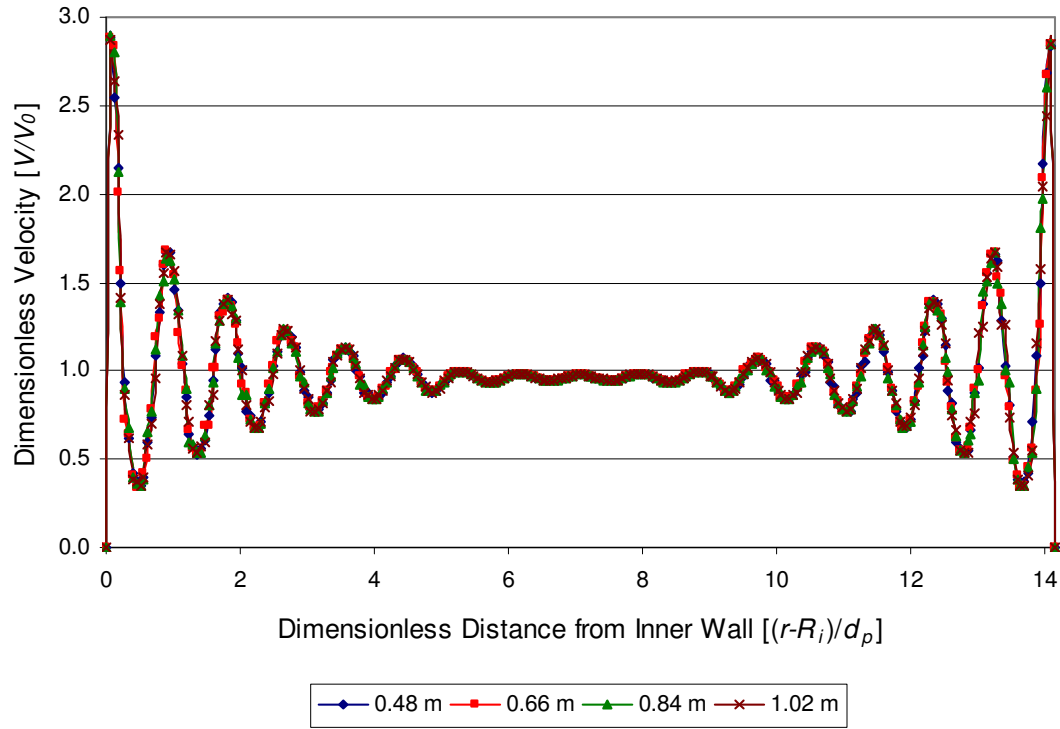


Figure 5-18: Velocity distribution through bed's bulk region

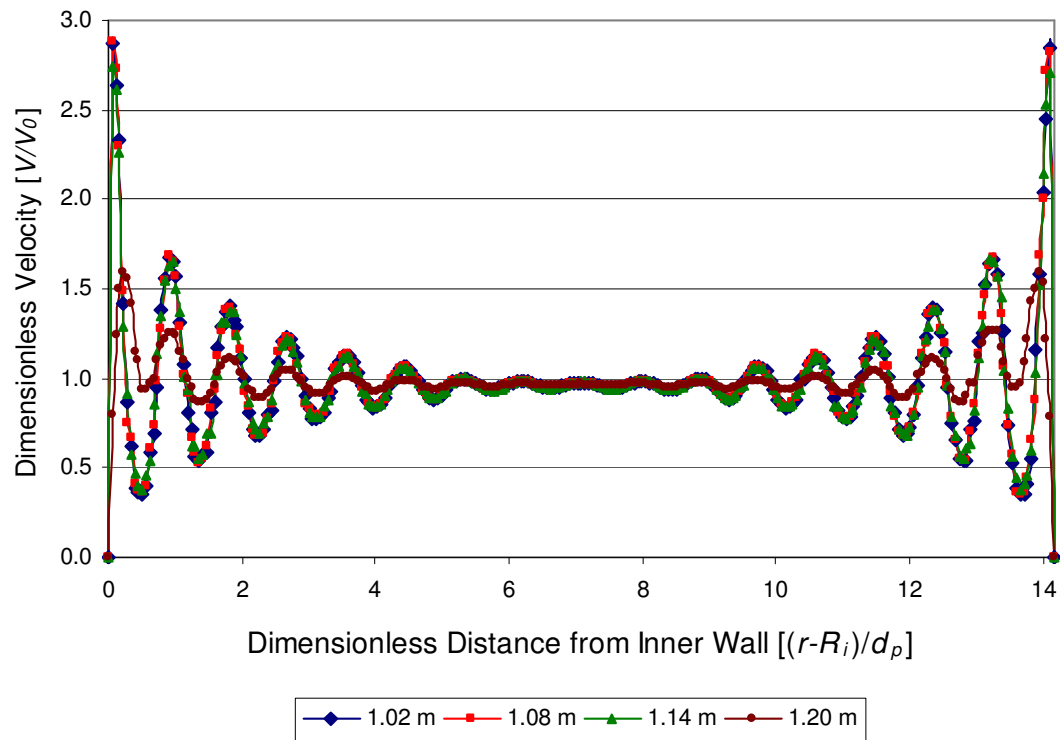


Figure 5-19: Velocity distribution through bed's outlet region

The fluid redistribution in the outlet region of the bed can be seen in Figure 5-19. The velocity profile remains constant up to a distance of one particle diameter from the bed exit. The amplitude of the velocity peaks is

reduced as the fluid moves through the bed's outlet region. The velocity peak, adjacent to the annulus walls, is moved slightly inwards towards the centre of the bed. In the model this fluid redistribution is dependant on the viscosity of the fluid. A greater degree of flow redistribution will be experienced by using a more viscous fluid and vice versa. For this reason, an effective viscosity model, which is dependant on the structure of the bed, is required.

Figure 5-20 shows the velocity profile that exists within the bed once the fluid flow is fully developed for a Reynolds number of $Re = 432$. This profile was obtained by averaging all the velocity profiles falling within $0.42 \text{ m} \leq z \leq 1.08 \text{ m}$.

In section 2.2 it was mentioned that Price (1968) found the normalised velocity distribution, through a packed bed, to be independent of Reynolds number for ranges of $1470 < Re < 4350$. Subagyo *et al.* (1997) found that the Reynolds number dependency, of the velocity profile, is no longer significant for Reynolds numbers larger than $Re \geq 500$. From the results of Subagyo *et al.* (1997), shown in Figure 2-2, very little difference can be observed between the flow profiles obtained at Reynolds numbers of $Re = 400$ and $Re = 500$. From the flow profiles of Giese *et al.* (1998), shown in Figure 2-3, very little differences can also be observed between the flow profiles obtained at Reynolds numbers of $Re = 103$ and $Re = 532$. Based on this, it is reasonable to assume that the velocity profile presented in Figure 5-20 remains the same for higher flow rates. The Reynolds number independency should be however verified by repeating the simulations at higher inlet velocities.

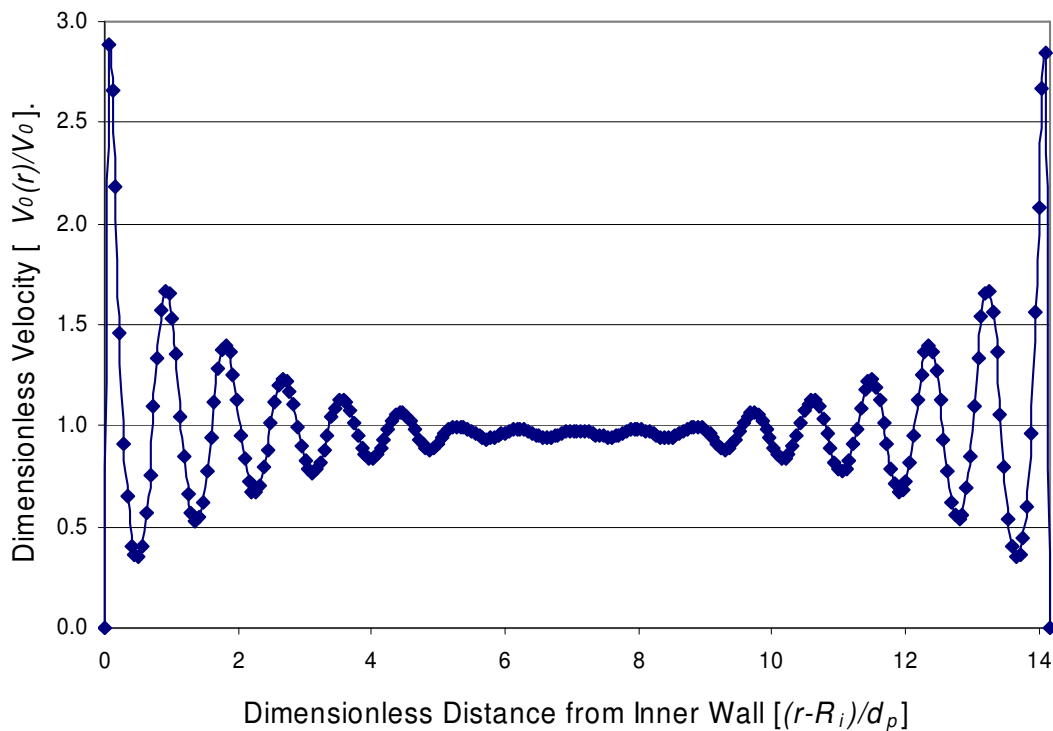


Figure 5-20: Fully developed velocity profile

The velocity profile is in good agreement with velocity profiles presented by other researchers (Giese *et al.* 1998 ; Bey & Eigenberger, 1997). The biggest difference is observed in velocity peaks adjacent to the wall. Giese found the magnitude of the peak to be roughly two and a half orders higher than the empty tube superficial velocity. The current model predicts a peak velocity that is of order 2.9 higher than the superficial velocity. As stated in section 5.3.4, the effective viscosity has a significant influence on the velocity in the near wall region. The effective viscosity was adjusted in section 5.3 until the velocity peaks of the measured and simulated velocity profiles corresponded. Since a constant effective viscosity was used the fluid redistribution in the outlet region may have been over predicted. This implies that a much lower effective viscosity had to be employed to overcome the excessive fluid flow redistribution in the outlet region of the bed to allow the measured and simulated velocity profiles to show good agreement and as a result the velocity in the near wall region is over predicted. The need of a structure based effective viscosity model is thus emphasized by this fact.

The magnitude of the secondary velocity peaks is also lower than that found by Giese *et al.* (1998). Giese *et al.* (1998) used their own measurements of the porosity in the development of their model. Since it is impossible to determine the actual structure of the bed, used in the HTTU's velocity tests, the model is only as good as the correlations on which it is based. The higher secondary peaks, presented by Giese *et al.* (1998), may be due to porosity peaks that were higher than those predicted by the porosity correlation of Martin (1978). These higher porosity peaks would result in a lower porous resistance and allow for more fluid to pass through this region explaining the amplitude difference of secondary velocity peaks.

It can be concluded that the current model is capable of predicting the velocity distribution at a distance inside the bed where it can be assumed that the fluid flow is fully developed. By taking the structure of the bed, in the inlet and outlet regions of the bed into account, the development of the velocity profile over the inlet and the fluid flow redistribution, through the outlet, is also predicted. By assuming that the velocity distribution is symmetrical about the mid-plane, between the two annulus walls, the velocity profile can be presented by:

$$\frac{V_0(r)}{V_0} = \begin{cases} 51.34x & \text{for } x < 0.057 \\ 0.97 + 1.06e^{(-0.54x)} \cos(7.12x - 6.63) + 1.35e^{(-6.25x)} & \text{for } x \geq 0.057 \end{cases} \quad (5.20)$$

with

$$x = \begin{cases} \frac{r - R_i}{d_p} & \text{for } R_i \leq x \leq \frac{R_i + R_o}{2} \\ \frac{R_o - r}{d_p} & \text{for } \frac{R_i + R_o}{2} \leq x \leq R_o \end{cases} \quad (5.21)$$

Equation (5.20) was determined from Figure 5-20 by means of the least squares curve fitting method. The fitting procedure of equation (5.20) yielded a statistical R^2 value of $R^2 = 0.988$, which indicates a fairly good fit. Equation (5.20) however predicts a minimum velocity which is lower than that proposed by the simulation model. Using the Euclidean error norm the difference between the predicted and fitted velocity profiles was

calculated as 3.51%. This indicates a good fit between the predicted and fitted velocity curves. A comparison between the predicted and fitted velocity profiles can be seen in Figure 5-21.

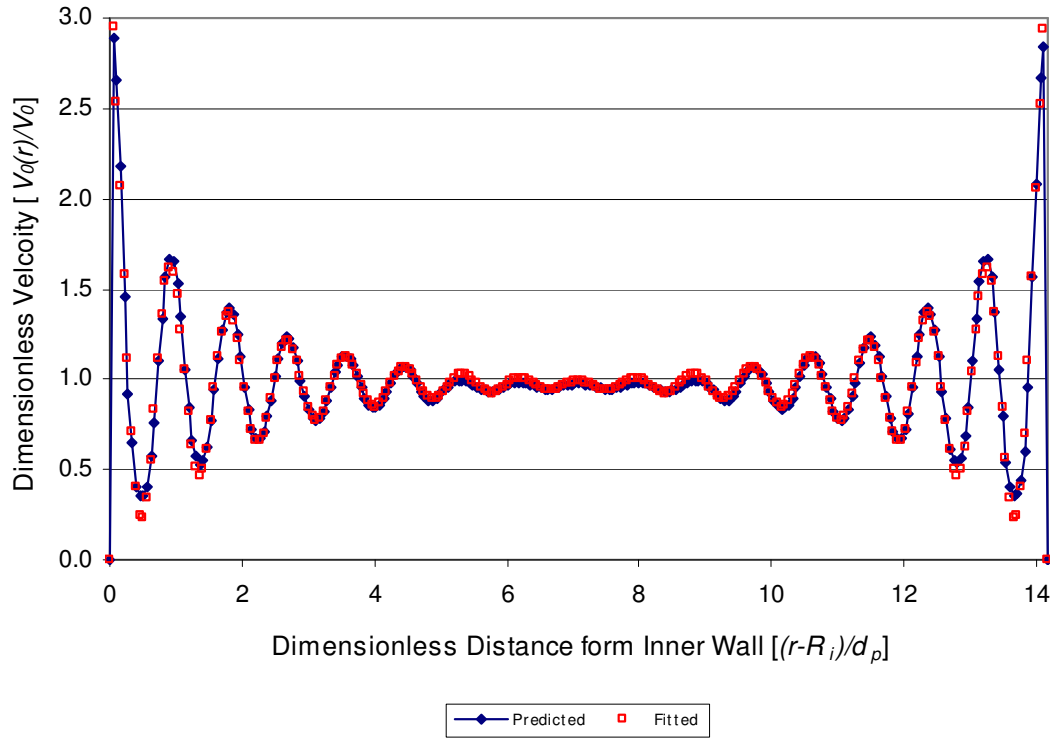


Figure 5-21: Comparison between predicted and fitted fully developed velocity profiles.

If it is assumed that the velocity profile is independent of the Reynolds number, for Reynolds numbers larger than $Re \geq 432$ rather than $Re \geq 500$ (Subagyo *et al.* 1997), equation (5.20) can be used to predict the fully developed velocity profile inside the bed.

The files for this simulation model can be found on the second disk at the back of the thesis.

5.5 Conclusion

This chapter dealt with the implicit modelling of the flow distribution in a packed bed. In modelling a packed bed in this manner the presence of the pores and spheres are taken into account implicitly through the employment of an empirical porosity correlation. These correlations only predict either the radial or axial variation in porosity. The porosity distribution in the bed outlet and inlet, where two walls disturb the packing, are however not predicted by these correlations.

It was found that the porosity distribution in the outlet region of the bed could be described by letting the porosity, predicted by the radial porosity variation correlation, increase linearly to unity over the last sphere diameter of the bed. The correlation describing the porosity distribution in this region is given by equation (5.1)

. The porosity distribution in the inlet of the bed, near the container and bed support walls, was best described by a weighted average of the axial and radial porosities as described in equation (5.2).

It was uncertain which porosity correlation and effective viscosity model was best suited to the implicit modelling of a packed bed. Closure regarding these uncertainties was obtained through a series of implicit bed simulations of the HTTU's packed bed. It was found that using the porosity correlation, proposed by Martin (1978), the KTA pressure drop correlation (1981) and the effective viscosity model of Giese *et al.* (1998), adjusted by a factor of 0.8, for a Reynolds number of $Re=432$ and no larger Reynolds number yielded a velocity profile that was in good agreement with the experimental velocity profiles.

This modelling methodology was applied to an annular packed bed with an inner and outer radius of $R_i = 0.3$ m and $R_o = 1.15$ m and a bed length of $L = 1.2$ m. The fluid flow through the bed corresponded to a Reynolds number of $Re=432$. A significant amount of flow redistribution is observed in the bed outlet ($L - d_p < z \leq L$). The basic shape of the velocity profile is established within one particle diameter from entering the bed. The amplitude of the velocity peaks increases in magnitude over the inlet region of the packed bed until the flow is fully developed. Once the fluid flow is fully developed, the velocity distribution is independent of bed height for $5d_p < z < L - d_p$ and is described by equation (5.20).

The next chapter provides an executive summary of the study, conclusions drawn from the study and recommendations for future work.

Chapter 6

Conclusions & Recommendations

6.1 *Executive summary*

This study dealt with the investigation into the velocity distribution through an annular bed packed randomly with spheres. Most simulation models, where the spheres and pores are modelled implicitly, only predict the velocity distribution at a distance inside the bed where it is assumed that the fluid flow is fully developed. In simulation models where the spheres and pores are modelled explicitly the models are confined to a few particles due to the huge computation resource requirements associated with these model's meshes. The main purpose of the study was to develop a simulation model capable of predicting the development of the velocity profile through the inlet and outlet regions of the bed along with the velocity profile inside the bed once the fluid flow was fully developed by using a commercial RANS CFD code.

Firstly, the velocity distribution above the annular packed bed of the HTTU, for a variety of mass flow rates, was investigated experimentally. Despite some shortcomings of the measurement instrumentation, the velocity profiles showed good agreement with one another. The presence of wall channelling is clearly visible in the velocity profiles. The profiles also indicate that the velocity distribution is independent of the mass flow rate through the bed.

The velocity profiles did however not represent the axial velocity component since the CTA measured the resultant of the axial and radial velocity components. At low mass flow rates this was visible as the integration of the velocity profiles, over the entire annular region, yielded mass flow rates higher than the actual test mass flow rates.

In order to obtain a better understanding of the distribution of the axial velocity vector component, the relation between axial velocity component and the resultant of the axial and radial velocity components was investigated numerically using the commercial RANS CFD code STAR-CCM+[®]. The spheres and pores were modelled explicitly and the stagnant and low flow regions around the contact points between spheres were removed and replaced by cylinders. In an independent study it was found that this approach significantly reduced the computation resource requirements of the mesh without noticeably affecting the flow distribution downstream of the spheres. A relation was established between the axial velocity component and the resultant of the axial and radial velocity components. This relation was then employed to extract the axial velocity vector component from the measured velocities. Integration of these modified velocity profiles yielded a mass flow rate that was in close agreement to the actual mass flow rate that was used during the test.

Since the explicit modelling of an entire packed bed is currently not feasible, the annular packed bed of the HTTU was modelled implicitly. This approach calls for an empirical correlation that describes the porosity of the bed and a pressure drop correlation representing the resistance to the flow from the spheres. The porosity correlations only describe the variation in porosity in the radial and axial direction. No correlation describing the porosity in the inlet and outlet regions could be found. In a separate study it was established that the porosity in the inlet region could be described by means of a weighted average of the axial and radial porosity. The porosity distribution in the outlet region was best described by letting the radial porosity increase linearly to unity in the axial direction over a distance of one sphere diameter from the bed outlet.

The modified velocity profile, at a mass flow rate of 0.5 kg/s, was used in verifying the simulation model. The model however over predicted the velocity peaks in the near wall region. For this reason an effective viscosity model was employed to model the fluid flow in the near wall region. The effective viscosity caused the near wall velocity peaks to decrease in amplitude and to be shifted inwards to the centre of the annulus. The value of the effective viscosity was adjusted until a good agreement between the predicted and experimentally adjusted velocity profiles were achieved.

Due to the complex inlet geometry of the HTTU no significant information regarding the development of the velocity profile over the inlet region of the bed could be established. For this reason the same modelling approach was used in a simulation model of an annular packed bed with a uniform velocity inlet. From the simulation model the manner in which the velocity profile develops over the in- and outlet region of the bed was established. The velocity profile inside the bed, once the flow field is fully developed, was also determined along with the region inside the bed where the flow field is fully developed. The fully developed velocity profile compared favourably with other profiles listed in the literature.

6.2 Conclusions

From the experimental investigation into the velocity distribution it can be concluded that the velocity profile, both in- and outside the bed, is independent of the mass flow rate for a Reynolds number range of $438 < Re < 3453$.

The greatest benefit of the current simulation model is that it is not limited to exclusively predicting the fully developed velocity profile inside the bed although the models for the inlet and outlet regions could not be validated explicitly. The current model is also capable of predicting the development of the velocity profile over the in- and outlet regions of the bed. The basic shape of the velocity profile is established almost immediately once the fluid enters the bed. The amplitude of the maximum and minimum velocity peaks however increases and decreases in magnitude over a distance of five sphere diameters from the bed inlet until the profile is fully developed. The profile remains unaltered from here on out up to a distance of one sphere

diameter from the outlet of the bed. In the outlet region of the bed a significant amount of fluid redistribution occurs. The amplitude of the velocity peaks are reduced and shifted inwards as the fluid exits the bed.

The current simulation model will be of great use in simulation models where fluid circulation in the bed due to natural convection is under investigation.

6.3 Recommendations for future work

In the current simulation model a number of assumptions were made which may influence the accuracy of the simulation model. For this reason the following improvements are recommended.

The current radial porosity correlations that had been used were derived for cylindrical packed beds. These correlations were modified to be symmetrical around the centre of the annulus. No correlations describing the variation in the porosity for an annular packed bed exist. Of particular interest is the variation in porosity near the inner annulus wall. Here the packing is situated on the outside of a curved surface and not on the inside of a curved surface such as the outer annulus wall and cylindrical bed for which the porosity correlations have been derived. A thorough investigation into the porosity variation of a bed on the outside of a convex surface is thus required.

In the simulation model the porosity in the inlet region of the bed, where two walls disturb the packing structure, was approximated as a weighted average of the axial and radial porosity distributions. The averaging process yielded wall porosities that were less than unity close to the contact point between the two walls. For this reason a thorough investigation into the porosity distribution and a correlation describing the porosity distribution in this region is required.

In the simulation model the KTA (1981) pressure drop correlation was applied to porosities for which the correlation is no longer valid. These regions are mainly found close to the wall where the velocity was over predicted without the use of an effective viscosity model. This may be because the resistance, predicted by the correlation, was too low and allowed for more fluid to pass through these regions. For this reason it is recommended that the correlation be expanded to include a wider range of porosities for which it is valid. This would also eliminate the need for an effective viscosity model to model the fluid flow in the near wall region.

An effective viscosity model was employed in the simulation model to model the fluid flow in the near wall region. It has been well established that the effective viscosity only affects the velocity distribution in the near wall region. It does however affect the pressure drop across the bed with a higher effective viscosity resulting in a higher predicted pressure drop. The current effective viscosity model is based on a single value that is applied to the entire bed. It does not account for the structure of the bed. For this reason it is recommended that work should be done to establish an effective viscosity model that is dependent on the porosity to ensure that

the fluid flow in the near wall region is simulated correctly and does not allow the pressure drop to be over predicted.

The current model only investigates the velocity distribution through the bed under forced convective, isothermal fluid flow conditions. M-Tech Industrial (Pty.) Ltd. has natural convection test data for the HTTU. For this reason it is recommended to investigate the fluid circulation in the bed under natural convective fluid flow conditions. This will also serve as good test for the inlet and outlet region models.

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