



A CFD model of the thermal hydraulic behaviour of the HTTU annular packed bed

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PREFACE

Acknowledgements

The completion of this work has been a few years in the making. What I've seen happen in my own life and world events during this time, can only be described as an adventure. I have kept working and chiselling away at the pages and now, somehow, managed to stand at the end.

The end of this thesis I mean.

At the time of writing, one should be careful with such words. We have felt our world turned upside down through a global pandemic and seen countries pushed to the edge of nuclear war. This work, then, attests to the peaceful use of the atom, or whichever new subatomic *atomos* might be found to constitute this ultimate form of energy.

I can say that, as with all good things, it simply takes time to accomplish. Time and effort. Truth be told, there have been many challenges and setbacks. I remember when I first came across new publications that were touching on what my initial simulation goals were. These challenges seemed to move the goal posts further and further along. The lesson is then that it is truly about the journey, and not the end.

As this work comes to an end, so there will be many new beginnings, new opportunities. When I started, it would be explained that one (the 'typical student' – as if there is such a creature) completes one degree after the other: a Master's student enrolls for a PhD; a Doctorate should be finished in x amount of time or *usually a student completes their study and then starts work*. "Typically, one would..." is in fact not 'typical' or the norm – it is not a rule as such: the average of a situation comes about as a function of considering each non-typical datapoint, each outlier...

Possibility is like standing in a palace filled with doors, rather than a long corridor with one door at the end. And the floor plan has not been laid out to aid navigation; some hidden paths connect rooms that were perhaps even previously visited, trap doors stifle your pace, the floorboards creak and might give way. But, now, for this journey, there is indeed a light at the end of this particular corridor: the final door of this adventure.

And so, there is a journey for everyone. Be sure to tread carefully, surely, truly, but most importantly – forward. Every step brings one closer to the destination, even if it takes you on the longer, scenic route. You will come to your destination – stronger and wiser.

But this work, this journey, was not possible on my own and therefore many heartfelt thanks are due:

First and foremost, to my wife, Lena – the person I've chosen to share my life with and therefore the same challenges of completing this study part-time. Your kind words, caring and love have carried me through the most difficult parts of this work (and life). Thank you for your support and your understanding, and for most of all, believing in me! Without the sacrifices you have made, this work could not have been possible. Thank you also to my parents-in-law for their encouragement.

To my parents, for their encouragement and support throughout my upbringing, for which a mere thank you could never recount, and even now. I am truly grateful to have had the opportunity to study, learn and work. It would not have been possible without parents who had the faith to believe in me, the insight to motivate me and the wisdom to encourage me to be the best that I can. This work is dedicated to them and to those who never had the same opportunities.

To Prof Jat, for his endless reassuring patience, insights and guidance. Your deep understanding, calm demeanour and courageous approach to large and daunting tasks have been an inspiration. That, combined with the right amount of humour, has made this work as interesting as it was enjoyable. I could not have done this without you.

To all my friends, relatives and colleagues who have encouraged me and asked with sympathy, empathy or just curiosity. Each word of encouragement has helped.

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Last but not least, Christiaan de Wet and the team at Aerotherm for their technical support on CD Adapco and eventually Siemens Star-CCM+. Your support towards the end of this study has been just as diligent as during my first questions that I sent back in 2014.

Vale et virtute ac ratione utare sub auspiciis Imperii aeterni.

ALICUBI GALLIAE BELGICAE NOVEMBRI MENSE, ANNO DOMINI MMXXIV.

LVX ET VERITAS



Information on Qualification

This thesis has been submitted, along with the research articles cited below, in fulfilment of the degree *Philosophiae Doctor* in Nuclear Engineering at the Potchefstroom campus of the North-West University.

Title: *A CFD model of the thermal hydraulic behaviour of the HTTU annular packed bed*

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Research Output

A list of published conference papers and journal articles submitted in relation to this study are:

1. Potgieter, M.C., Du Toit, C.G. (2024).
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Nuclear Engineering and Technology, 56(3):959-965. <https://doi.org/10.1016/j.net.2023.11.041>
2. Potgieter, M.C., Du Toit, C.G. (2023).
The porosity distribution in the HTTU annular packed bed of spheres.
Nuclear Engineering and Design, 402:112124. <https://doi.org/10.1016/j.nucengdes.2022.112124>
3. Potgieter, M.C., Du Toit, C.G. & Kruger, J.-H. (2016a).
A fully integrated 3D CFD model of the flow and heat transfer in a packed bed reactor.
In: *Conference proceedings*. 8th International Topical Meeting on High Temperature Reactor Technology (HTR 2016), Las Vegas, NV, USA, 188.
4. Potgieter, M.C., Du Toit, C.G. & Kruger, J.-H. (2016b).
The evaluation of 3D CFD approaches to model the flow and heat transfer inside an unstructured bed of uniform spheres.
In: *Conference proceedings*. 10th South African Conference on Computational and Applied Mechanics (SACAM 2016), Potchefstroom, South Africa.

Abstract

Very high temperature gas-cooled reactors (VHTGRs) could play a pivotal role in the future of the energy transition away from carbon as several industries relying on high temperature process heat and steam as input. VHTGR plants offer a zero-emission thermal energy source, compared to direct heat from the combustion of coal, oil and gas or indirectly from electricity generated at a lower efficiency from the same sources. Compared to renewables, nuclear has unmatched availability for base load supply and is therefore seen as an important component towards energy sustainability (World Nuclear Association, 2024). Several VHTGR designs have been proposed based on a pebble bed core consisting of spherical fuel elements. Such pebble bed reactors (PBRs) have been built in the past showing promising results. In their design and operation, however, it was noted that there is a large degree of uncertainty around predicted and observed temperatures.

Modern modelling techniques such as computational fluid dynamics (CFD) aim to solve modelling issues of the past, but often come with a large computational expense. Integral effects tests contribute not only to the qualification of next-generation designs but also to the validation of codes including CFD models. The High Temperature Test Unit (HTTU) was an integral effects test of the thermal conduction, radiation and convection in an annular pebble bed, based on the PBMR-400 design.

This study presents two approaches to the numerical modelling of the pebble bed of the HTTU experiment in the finite volume CFD code, Star-CCM+: a coarse mesh full model of the bed using a representative porous medium, and a fine mesh model of a section of the bed with discrete geometry of resolved solid spheres and flow domain. The annular packed bed geometry was generated using a discrete element method (DEM) code ESSS Rocky, with the geometry extracted in the case of the discrete geometry, and a separate method used to obtain the radial and axial porosities used in the porous approach.

Results from experimental isothermal tests using nitrogen are used to validate the flow distribution and pressure drop of the two modelling approaches without heating. The models are then solved with forced convection, calibrated for the 1 kg/s 140 kW case and finally compared with the corresponding experimental results. A further comparison is done to other test conditions. Good agreement was found with differences less than measurement uncertainties. In the near-wall region the average relative error was found to be equal to 0.9% but in the bulk region the error reaches 38%.

Keywords: *HTTU; PBMR; HTGR; Pebble Bed; Packed bed; Porosity; Integral effects tests; Computational fluid dynamics; Discrete element method; Validation.*

Opsomming

In die toekoms van die energie-oorgang na minder koolstofverbruik kan hoëtemperatuur gas-verkoelde reaktore (HTGRs) 'n deurslaggewende rol in energie opwekking speel, soos verskeie industrieë, wat staat maak op hoë temperatuur proses hitte en stoom, wil weg beweeg van koolstof gebaseerde brandstowwe af. VHTGR aanlegte is 'n nul-uitlaatgas bron van termiese energie in vergelyking met direkte hitte wat deur die verbranding van steenkool, olie, gas of andersins indirek van elektrisiteit gegenereer word, teen 'n laer effektiwiteit, maar deur dieselfde kragbronne. In vergelyking met ander bronne van hernubare energie beskik kernkrag oor ongeëwenaarde beskikbaarheid vir 'n basis lading van kragtoevoer; en kan daarom dien as 'n belangrike mylpaal tot energie volhoubaarheid (World Nuclear Association, 2024). Menigte VHTGR ontwerpe wat voorgelê is, is gebaseer op die ontwerp van die korrelbedreaktor wat sferiese brandstof elemente bevat. Sulke korrelbedreaktore (PBRs) wat alreeds gebou was het belowende resultate opgelewer. Gedurende hulle ontwerp en die bedryf van die reaktore, was daar opgemerk dat 'n groot mate van onsekerheid heers tussen die verwagte en waargenome temperature.

Moderne modellerings tegnieke soos berekeningsvloeimeganika (CFD) poog om modellerings probleme van die verlede op te los, maar die berekeningskoste daarvan is hoog. Allesomvattende effekte-toetse dra by tot die kwalifikasie van die volgende generasie ontwerpe, asook die validasie van simulatie-kodes insluitende CFD. Die hoëtemperatuur toets eenheid (HTTU) was 'n allesomvattende effekte-toets vir die ondersoek van die termiese geleiding, straling en konveksie wat plaasvind in 'n annulêre korrelbed; soos gebaseer op die ontwerp van die PBMR-400.

Hierdie studie verteenwoordig twee benaderings vir die numeriese modellering van die HTTU-korrelbed eksperiment in die eindige-volume CFD kode Star-CCM+: 'n growwe rooster model van die volledige korrelbed met 'n verteenwoordigende poreuse medium, en 'n geval met fyn rooster waar slegs 'n segment van die korrelbed met diskrete geometrie van die soliede sfere gemodelleer word. Die gepakte annulêre korrelbed se geometrie was gegenereer deur die gebruik van 'n diskrete-element-metode (DEM) kode, genaamd ESSS Rocky. In die geval van die diskrete geometrie was die geometrie onttrek en vir die poreuse benadering was 'n aparte metode gebruik om die radiale en aksiale porositeite te verkry sodat dit gebruik kan word.

Die resultate van die isotermiese eksperimentele toetse met stikstof was gebruik om die vloieverdeling asook die drukval in die twee modelle sonder verhitting te valideer. Na afloop daarvan is beide modelle opgelos met geforseerde konveksie hitte-oordrag toestande, gekalibreer vir die 1 kg/s 140 kW geval en die resultate daarvan met dié van die ooreenstemmende eksperimentele gevalle vergelyk. 'n Verdere vergelyking is gedoen met ander toets-kondisies. Numeriese resultate het goed ooreengestem met die eksperimentele resultate met verskille in waardes kleiner as die meetinstrument-onsekerhede. In die nabye-wand gebied was die gemiddelde relatiewe fout minder as 0.9%, maar in die sentrale gebied bereik die verskille 'n waarde hoër as 38%.

Statement of Original Work

It is hereby stated and witnessed that the work contained in this thesis is the original work of the author, Marthinus Christiaan Potgieter.

The published article on which Chapter 3 is based is a co-authored work and permission to use the publication Potgieter & Du Toit (2023) in part and in full, is hereby granted by the co-author.

This statement is reflective of the copy submitted for examination on Wednesday 27 November 2024 and the consequent revised version containing corrections and modifications as per reviewers' comments to the satisfaction of the promotor, submitted on the date of signature below.

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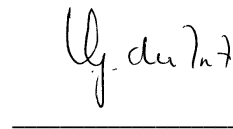


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Nomenclature

Abbreviations and Acronyms

1D	One-dimensional
2D	Two-dimensional
3D	Three-dimensional
ABTU	From the Russian АБТУ Атомная Блочная Транспортабельная Установка (nuclear block-transportable installation, or modular nuclear power plant)
ABTU-ts	From the Russian АБТУ-ц Атомная Базовая Технологическая Установка – Циркулирующая (Nuclear Basic Technological Plant – Circulating, referring to spherical fuel elements being circulated)
AHTR	Advanced High Temperature Reactor
AP-HTTF	A numerically packed bed of the HTTU, generated using PFC3D and <i>AP</i> referring to the author of the work <i>Alexander Polson</i>
ANL	Argonne National Laboratory
ASME	The American Society of Mechanical Engineers
AVR	<i>Arbeitsgemeinschaft-Versuchs-Reaktor</i> (Research Reactor Working Group, a research reactor in the former West Germany)
BCC	Body-centred-cubic
BETS	Braiding Effects Test Sections (experiment at NWU)
CFD	Computational Fluid Dynamics (numerical method)
CHPC	Centre for High-Performance Computing (South Africa)
CPU	Central Processing Unit
DDR	Double Data Rate computer memory
DEM	Discrete Element Method (or Modelling, numerical method)
DNS	Direct Numerical Solution (resolved turbulence)
DST	Department of Science and Technology (South Africa)
ESKOM	Electricity Supply Commission (South Africa)
ESM	Expanding System Method, grid-based numerical method, so-called by the authors in Hao, <i>et al.</i> (2022).
ESSS	Engineering Simulation and Scientific Software (a Brazilian multinational company)

FCC	Face-centred-cubic
GIF	Generation IV International Forum
GNU GPL	GNU-project General Public Licenses
GPU	Graphics Processing Unit
HPC	High Performance Computer (or Computing)
HPTU	High Pressure Test Unit (experiment at the NWU)
HTGR	High Temperature Gas-cooled Reactor (also HTGCR)
HTMR	High Temperature Modular pebble bed nuclear Reactor
HTR	High Temperature Reactor, or <i>Hochtemperaturreaktor</i>
HTR-PM	High-Temperature gas-cooled Reactor Pebble-bed Module
HTR-PROTEUS	Pebble bed core loading of the zero-power PROTEUS research reactor at PSI
HTTF	High-Temperature Test Facility (facility at the NWU)
HTTU	High Temperature Test Unit (experiment at the NWU HTTF)
I/O	Input / Output, reading and writing of computer code data
IAEA	The International Atomic Energy Agency
INET	Institute of Nuclear and New Energy Technology (at Tsinghua University in Beijing, China)
ISO	<i>Organisation Internationale de Normalisation</i> , International Organization for Standardization
KAERI	Korea Atomic Energy Research Institute
KS	Kugeler-Schulten (referring to the Nusselt number correlation in the KTA standards)
KTA	<i>Kerntechnischer Ausschuss</i> (The Nuclear Safety Standards Commission, of the Federal Republic of Germany, also used in reference to their standards documents)
LBM	Lattice Boltzmann Method (numerical method)
LES	Large Eddy Simulation (turbulence model)
LOCA	Loss Of Coolant Accident
LOFC ATWS	Loss of Forced Coolant Anticipated Transient Without Scram
MIT	Massachusetts Institute of Technology
MPBR	MIT Pebble Bed Reactor

MSUC	Multi-Sphere Unit Cell (model for effective thermal conductivity)
NEA	The Nuclear Energy Agency, organized under OECD
NICIS	National Integrated Cyber Infrastructure System (South Africa)
NQA-1	ASME Nuclear Quality Assurance (referring to certification)
NRF	National Research Foundation (South Africa)
NVMe	Non-Volatile Memory express
NWTCTF	Near-wall Thermal Conductivity Test Facility (experiment at the NWU)
NWU	The North-West University (in South Africa)
OECD	The Organisation for Economic Co-operation and Development
OL	Overlap
PBMM	Pebble Bed Micro Model (experiment at NWU)
PBMR	Pebble Bed Modular Reactor (referring to the company)
PBMR-400	Pebble Bed Modular Reactor 400 MWth (referring to the design)
PBR	Pebble Bed Reactor
PSI	Pual Scherrer Institut
PTV	particle tracking velocimetry
RAM	Random Access Memory
RANS	Reynolds-averaged Navier-Stokes (turbulence model)
RSM	Reynolds-averaged Stress Model (turbulence model)
SANA	<i>Selbsttätigen Nachwärmeabfuhr</i> (Automatic Heat Removal, a plant cooldown experiment at Research Centre Jülich)
SARCHI	South African Research Chairs Initiative
sCFD	systems-CFD
SGL	SIGRI Great Lakes, referring to a merger of companies forming the SGL Group – a carbon and graphite manufacturing company
SOC	State-Owned Company (in South Africa)
SSD	Solid State Drive
TF-PBEC	Test Facility Pebble Bed Equivalent Conductivity (experiment at INET)
TF-PBF3D	Test Facility Pebble Flow 3D (experiment at INET)

THTR	<i>Thorium Hochtemperatur-Reaktor</i> (Thorium High-Temperature Reactor, a prototype reactor in the former West Germany utilising mixed Uranium-Thorium fuel)
TRISO	TRi-structural ISOtropic
UCAR	Carbon products division of <i>Union Carbide</i> , now known as <i>GrafTech International</i> (US multinational company)
UDF	User-Defined Function
VG	Variation of VGR
VGM	Variation of VGR
VGR	From the Russian ВГР Высокотемпературный Гелиевый Реактор (High-temperature Helium Reactor) or Высокотемпературный Газоохлаждаемый Реактор (High-Temperature Gas-cooled Reactor), depending on sources
VHTGR	Very High-Temperature Gas-cooled Reactor
VHTR	Very-High-Temperature Reactor
ZBS	Zehner-Bauer-Schlünder (updated model for effective thermal conductivity)
ZS	Zehner-Schlünder (model for effective thermal conductivity)
(Pty) Ltd.	A Proprietary company with Limited liability (corporate law in certain countries e.g. South Africa, Australia and Hong Kong)

Alpha-numeric symbols

∂	partial differential symbol
A	area
c	damping coefficient
c_p	specific heat capacity
D	bed diameter
d	particle diameter
E	material Young's modulus
e	material restitution coefficient
F	resultant force

I	moment of inertia
k	spring stiffness coefficient, turbulent kinetic energy
k_{eff}	subscript <i>reactivity</i> : the effective neutron multiplication factor; subscript <i>conductivity</i> : the effective thermal conductivity
k - ε	a two-equation turbulence model with k and ε terms
L, l	length
m	mass of a particle
Nu	Nusselt number
$\mathbf{n}$	normal vector
N_2	Nitrogen (in diatomic form, denoted by the subscript 2)
Pr	Prandtl number
p	pressure
R	sphere radius
Re	Reynolds number
r	radial coordinate
S	arc length
$\mathbf{s}$	tangential vector
t	time
$\mathbf{v}$	translational velocity
y	radial distance
y^+	dimensionless parameter (used in CFD to denote distance from first cell to wall)
z	axial coordinate

Greek symbols

Δ	change (e.g. pressure change or height difference)
δ	displacement
ε	porosity; turbulence dissipation rate
$\bar{\varepsilon}$	average porosity
η	damping ratio
θ	azimuthal angle in radians
μ	skewness, dynamic viscosity
μ_s	coefficient of friction
v	velocity
π	the numerical constant Pi
σ	standard deviation
ς	relative displacement
τ	resultant torque
ω	angular velocity

Subscripts

I	inner limit
2	outer limit
2	to denote a diatomic substance as in N_2 diatomic nitrogen
b	bulk
c	contact
g	gravitation
h	upper axial limit
Hz	Hertzian

i	inner; position variable
j	position variable
ij	from i to j
l	lower axial limit
max	maximum
N	Normal
nc	non-contact
o	outer
p	at constant pressure, as in c_p
p	particle
S	tangential (Sliding)
s	superficial
ε	porosity

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1. INTRODUCTION

1.1. Background to the Study

1.1.1. High Temperature Reactors

A High Temperature Reactor (HTR, also *Hochtemperaturreaktor* in German) is a type of gas-cooled and graphite-moderated reactor (also HTGR or HTGCR), capable of reaching coolant temperatures at the core outlet of 750 °C or more (Kugeler & Schulten, 1989). This high temperature thermal output could serve industrial applications requiring high temperature steam or direct process heat or for conventional generation of electrical energy and several HTR reactors have already been designed, built and operated successfully.

The fuel considered in modern designs consists of layered kernels of so-called TRi-structural ISOtropic (TRISO) particle fuel, embedded in a graphite matrix and encased with a final graphite shell forming a spherical fuel element or pebble (see Figure 1.1). The presence of a high graphite-to-fuel mass which is widely dispersed volumetrically, results in a highly thermal neutron spectrum with relatively low thermal energy density and furthermore, because of a strongly negative temperature feedback coefficient, it is considered an accident-detering fuel (Brähler, *et al.*, 2012).

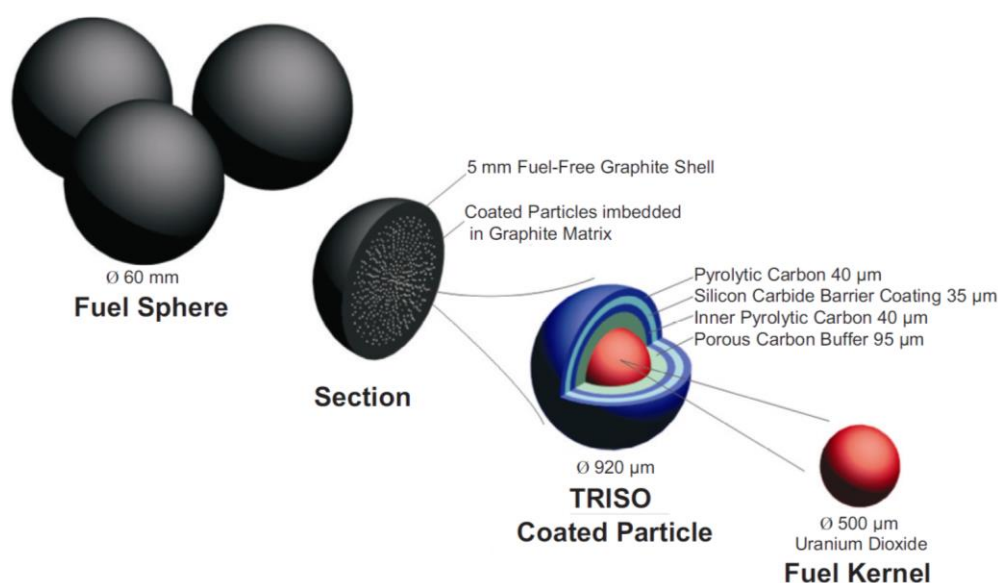


Figure 1.1: Spherical fuel elements or “pebbles” the source of thermal energy in pebble bed reactors (Idaho National Laboratory, 2010).

1.1.2. Very-High Temperature Reactors

The Very-High-Temperature Reactor (VHTR) is a proposed future graphite-moderated reactor based on high temperature inert helium gas as coolant. Advantageous characteristics include very high core outlet temperatures of 950 °C and beyond, high fuel burn-up and an inert single-phase primary coolant (Nuclear Energy Agency (NEA), 2014).

The Generation IV International Forum (abbreviated as GIF) lists the VHTR as one of 6 candidate Gen IV nuclear systems on its technical roadmap (Generation IV International Forum, 2024), with a focus on capabilities resulting from very high outlet temperatures useful in applications ranging from hydrogen production (Elder & Allen, 2009) or high-grade process heat for demanding industries, to direct cycle electricity generation where primary coolant is used directly with resulting high efficiencies.

Currently two core configurations are considered: a prismatic block design, and a pebble bed design. The difference between these are both the core and fuel geometry.

- In **Prismatic Block** reactors: the fuel of coated TRISO microspheres is contained in a cylindrical graphite matrix element, which is placed within hexagonal block fuel assemblies which in turn are stacked and placed in a hexagonal arrangement radially to form a critical core.
- In **Pebble Bed** reactors: the same TRISO fuel is contained in a graphite matrix forming a spherical fuel element covered with another layer of only graphite, also called a pebble; the core geometry consists of an elongated cylindrical or annular space filled with thousands of pebbles.

1.1.3. Pebble Bed designs

The focus of this study is centred on pebble bed reactors (PBRs), and in particular the thermal hydraulics. The concept of a gas-cooled reactor with “unconformable units or lumps” of moderator and fuel, was first conceived in 1945 by Farrington Daniels (Daniels, 1957). There are only three PBR designs that have been operated in the past and one which is currently in operation.

During the 1960's the *Arbeitsgemeinschaft-Versuchs-Reaktor* (AVR) was the first *Kugel¹-schüttungen* (“ball fillings”) or pebble bed nuclear reactor (Kugeler & Schulten, 1989). It was designed, constructed and operated as a 46 MWth experimental reactor generating 15 MWe of electricity in The Federal Republic of Germany (former West Germany), the success of which resulted in several further designs.

¹ The author finds the similarity between “Kugel” and the last name of Prof. Dr.-Ing. Kurt Kugeler, a pioneer in the field, a happy coincidence.

Between 1972 and 1984, the *Thorium Hochtemperatur-Reaktor* (THTR) was constructed and commissioned. It had a design power of 750 MWth and produced 300 MWe. Both the AVR and THTR-300 have been decommissioned and partially dismantled.

The third PBR to have been operated and the operational at the turn of the century and the is the Chinese HTR-10 (Wu, *et al.*, 2002). An experimental reactor designed according to German specifications and built in China it was first operational in 1995 and is currently in long-term shutdown. It was designed to produce electricity through an indirect steam cycle with a power rating of 10 MWth and 3 MWe (Xu, 2002).

As a first-of-a-kind demonstrator, the Chinese-designed HTR-PM, classified as an SMR, is the only currently operational pebble bed reactor design in the world. The Shidao Bay-1 reactor in Weihai, China consists of two 250 MWth reactors with steam generators connected to a single steam turbine to produce 200 MWe (IAEA, 2024). Construction started in 2012 and first criticality was achieved on 12 September 2021. First connected to the grid at the end of 2021, the plant has been commercially operational since 6 December 2023, a milestone for PBRs.

Several PBR concepts have been designed in the past but never constructed, with the designs considered abandoned currently. These include the HTR-*modul* (or module), HTR-100, and HTR-500 in Germany (Kugeler & Schulten, 1989), the experimental ABTU-15, pilot plant ABTU-ts-50 with a VGR-50 prototype reactor (Rosatom, 2023), VG-400 and VGM-200 of the Russian Federation (Golovko, *et al.*, 1996), the PBMR-400 in South Africa (Pebble Bed Modular Reactor SOC Ltd., 2017) as well as the MIT Pebble Bed Reactor (MPBR) in the United States of America (Kadav, 2007).

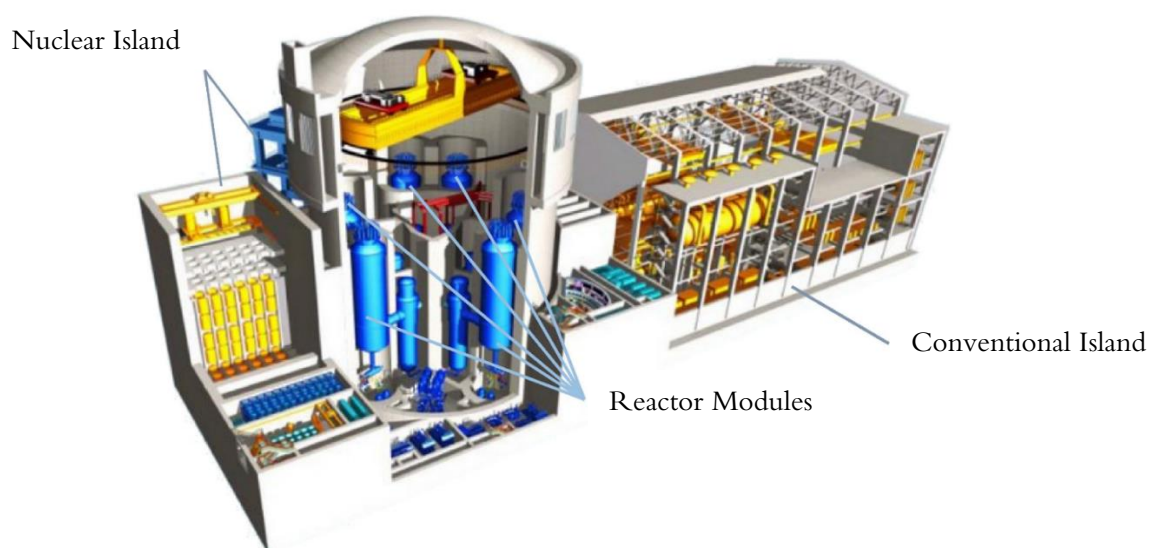


Figure 1.2: Diagram of the HTR-PM600 plant concept, with six reactors and three steam generators shown (Dong, *et al.*, 2018).

Other PBR designs which are currently in development are the X-energy Xe-100 (World Nuclear News, 2022) in the USA, the Huaneng Group HTR-PM600 in China (Dong, *et al.*, 2018), and the HTMR-100 of Stratek Global and AHTR 100 of ESKOM in South Africa (Nicholls, 2017).

1.1.4. Experimental facilities in support of PBR designs

In support of the development of PBRs, several experimental facilities are constructed to assist in the characterisation of physical phenomena related to the coolant flow and fuel heat transfer, form a basis for qualification of technology as well as generate data for the verification and validation of numerical codes – all towards furthering licensing efforts.

The facilities specifically constructed where data has been gathered concerning PBR thermal hydraulics are the SANA-1 test facility in Germany (Stöcker & Nießen, 1997), the High Temperature Test Unit (HTTU) as part of the PBMR High Temperature Test Facility (HTTF) hosted at the North-West University in South Africa (Rousseau & Van Staden, 2008), and the TF-PBEC and TF-PBF3D facilities of the HTR-PM project in China (Zhang, *et al.*, 2016).

The data from these experiments are often cited in literature as being used for the validation of numerical codes of PBR thermal-hydraulics. Numerous other studies have been conducted on the flow, pressure drop and heat transfer in packed beds that are not considered here.

1.1.5. Numerical codes for the analysis of PBR thermal-hydraulics

A large number of codes have been developed that are extensively used in the design and analysis of PBRs. The codes range from detailed 3D codes (able to model PBR core flow paths and fuel elements explicitly), to simplified 3D/2D codes (using a porous media approach), to systems codes (1D and/or limited 2D or 3D). A summary and discussion of the applicability of different codes is presented in Chapter 2 of this study.

In particular, this study builds on previous studies that were based on aspects of the HTTU experiments and focuses on the explicit modelling of the forced convection transfer experiments performed in the HTTU accounting for the solid pebbles, gas flow paths and the radiative, conductive and convective heat transfer. Two modelling approaches are discussed: using a fully explicit geometry, thereby resolving the solid pebble geometry; and using a porous medium approach, both with a finite-volume method 3D CFD solver.

1.2. Problem Statement and Scope

1.2.1. Research problem statement

To develop a fully integrated model of a packed pebble bed using a discrete numerical approach, in order to investigate the flow and heat transfer characteristics, to obtain a better understanding of the underlying phenomena and thereby validate, expand and improve upon existing predictions made by analytical methods.

1.2.2. Scope

The scope of this study is limited firstly by the design of the HTTU experiment and secondly by the operational envelope of the forced convective tests that were considered. Although natural convection tests were done in the HTTU using helium as well as near-vacuum tests to determine the effective thermal conductivity (Rousseau, *et al.*, 2014) all forced convection tests were only performed with nitrogen. As the facility was also not nuclear, the focus of the study is also limited to the thermal-hydraulics and does not consider the neutronics of PBRs.

1.3. Objectives and Motivation

The objective of this study is to present two approaches to modelling the integral heat transfer of the High Temperature Test Unit annular packed bed under forced convection using Computational Fluid Dynamics and compare the results with that of the experiment, taking uncertainty into account as a preliminary validation.

As is shown from the review of literature, there has not been a published study on an annular packed bed experiment under forced convection and therefore previously proposed modelling approaches have not been validated. Further motivation is to understand the phenomena that led to higher-than-expected temperatures from that predicted by analytical methods but observed in melt strips (as shown in Figure 2.11 in Section 2.2.4).

1.3.1. Unique contribution of this study

The unique contribution of this study is therefore the first time that the HTTU integral heat transfer is modelled with CFD and could lend further insights into heat transport in annular packed beds and the validity of assumptions and bringing different aspect that have been studied separately, together.

1.3.2. Building on previous studies

This work builds upon previous studies done at the School of Mechanical and Nuclear Engineering and through the DST/NRF SARCHI Research Chair in Nuclear Engineering at the North-West University.

Reyneke (2009) investigated the isothermal velocity profiles above the HTTU bed using discrete geometry and Reynolds-Averaged Navier-Stokes (RANS) CFD in order to apply a porous geometry that recreates similar profiles. Van Antwerpen (2009) modelled the effective thermal conductivity in the near wall region of the HTTU packed bed under nitrogen at near-vacuum (10 kPa). In the work by Preller (2011) LES was applied to model the flow and tortuosity in a section of the bulk region in a randomly packed bed as well as structured beds. A discrete element method (DEM) was utilised to generate representative cylindrical packed beds with small diameter to particle diameter ratios and analysed under isothermal flow conditions with RANS CFD in the work by Van der Merwe (2014). In this work (Van der Merwe, 2014) focus was given on the contact treatment between discrete spheres that is compatible with high quality CFD meshing in order to capture flows but minimise cell count. Vermaak (2019) performed a validation of the model of Preller (2011) applied to a structured bed to analyse the thermal dispersion in a structured bed using LED CFD. Van Loggerenberg (2020) built on previous work by conducting k - ϵ RANS CFD investigations of the pressure drop through the HPTU structured packed bed, comparing the numerical and experimental results to that of semi-analytical methods in literature. Focussing on only conductive heat transfer with contact modelling, De Beer (2021) used discrete geometry CFD in order to characterise the effective thermal conductivity observed in the structured bed in the Near-wall Thermal Conductivity Test Facility (NWTCTF). In a recent study, Bester (2022) presented a methodology to analyse the radial, axial and tangential porosity variations of an unstructured mono-sized pebble bed, compared it to previously known methods in literature and applied it to analyse the packed bed cylindrical core of the HTR-10.

1.4. Document Outline

As mentioned in the previous sub-section, there has not been an analysis done on the experimental data of a forced convective flow heated experiment in an annular packed bed configuration. To present this topic requires an explanation of the facility, literature and existing semi-analytical approaches. What this study explores is built around several main topics:

- i. Numerical modelling using either a discrete geometry or using a porous media approach, specifically applied to Computational Fluid Dynamics.
- ii. The use of Lagrangian Discrete Element Modelling to generate an unstructured packed bed geometry and assessing the validity of its application.
- iii. Forced flow velocity distribution and pressure drop through a randomly packed bed considered in an isothermal state.
- iv. Combined effects heat transfer under forced flow conditions.
- v. Validation and uncertainty qualification of the numerical results against measured values.

This work is structured in a way to gradually build on each of the topics to cover the scope of evaluating the numerical modelling of a heated packed annular bed forced convective flow experiment using CFD methods.

Firstly, the literature relevant to the full scope of the thesis is presented, evaluated and discussed in **Chapter 2**. This chapter focusses on the porous structure of PBRs, the experimental facilities used for integral heat transfer testing, numerical approaches such as the use of CFD and also references the analytical methods such as those included in the German KTA standards as accepted for analysis of the first generation of pebble bed reactors.

Chapter 3 is focussed on the numerical generation of a randomly packed bed using DEM, evaluating its porosity with the method of Bester & Du Toit (2022) and comparing this method with others found in literature. This chapter is based on the same work as already published by Potgieter & Du Toit (2023) and is re-published here with permission. The numerical bed of the HTTU annular packed bed is validated for use in further analyses, such as the discrete CFD flow and heat transfer models discussed in **Chapter 4**. This includes both a porous medium as well as discrete geometry numerical modelling approach. The detailed theoretical aspects, set-up of the numerical model and justification for the input boundary conditions and assumptions made is discussed herein.

The HTTU experimental campaign included isothermal forced flow runs, where the velocity distribution on the top of the bed was measured and these values are reported in **Chapter 5**. The detailed comparison of numerical results to the experimental measurements of the isothermal case is made later, in **Chapter 7**.

In **Chapter 6** the focus is on the electrically heated forced convective experimental runs. The resulting numerical results are eventually compared with the experimental values in **Chapter 7**, which includes a discussion of Verification and Validation efforts.

Along with the comparisons in **Chapter 7** the applicability and use of analytical methods is discussed and evaluated with other results, thereby coming back full circle to revisit the standards accepted in the past for the first generation of pebble bed reactors alongside the modern numerical methods presented.

Finally, the study concludes in **Chapter 8** with a summary of the work, its findings and the inferences drawn from the current results and further recommendations for future studies and potential application of the methods developed.

Any further detail relevant but not central to the study is provided in the **Appendices**, such as the HTTU test data and formulation of user defined functions.

End of Chapter

❧

2. LITERATURE OVERVIEW

This chapter outlines the literature relevant to the topics covered in the study: the physics of flow and conjugate heat transfer in a pebble bed, the experimental facilities used to characterise these phenomena and finally the application of numerical methods to model and analyse heat transfer under forced convection.

2.1. Geometry, Flow and Heat Transfer Phenomena

The flow and heat transfer characteristics of a pebble bed are defined by its packing structure. The unstructured arrangement results in voids allowing for flow and convection. This porous structure is not uniform in the vicinity of boundary walls and therefore has an influence on all other related parameters such as the flow dispersion or the reach of radiative heat transfer as examples. It is therefore apt to first discuss the porous structure and its characteristics.

2.1.1. Porous Structure

The porous structure of packed beds of various types and using different fill elements, including spheres, has been studied extensively in the chemical industry as well as for thermal storage solutions. In the nuclear industry, unstructured beds of uniform spheres have been characterised since the 1960's in different experiments to also investigate not only their porous structure but also the dynamic behaviour as the elements are mobile in the majority of PBR designs.

In cylindrical beds with static elements, the porosity distribution has been characterised by several authors, for example De Klerk (2003), Mueller (2012), and Du Toit (2019b). By analysing physical packings, it has been found that the porosity as function of radial distance to a wall is oscillatory. From inspection, it is clear that a structured packing with uniform contacts against a wall follows a porosity curve related to the geometry of the spherical volumes, starting from 1 and decreasing to a minimum, before again increasing, as does the space unoccupied by the volume of a sphere. This trend continues but in a damped way as moving away from the wall.

This characteristic is shown in Figure 2.1 where the porosity is overlain on an actual pebble bed geometry (that of the HTTU as used later in this study as the 'discrete approach') as well as the different parts typical of a cylindrical bed. The illustration in Figure 2.1 was made by taking a plane section through an actual randomly packed bed geometry per illustration of the different porous regions.

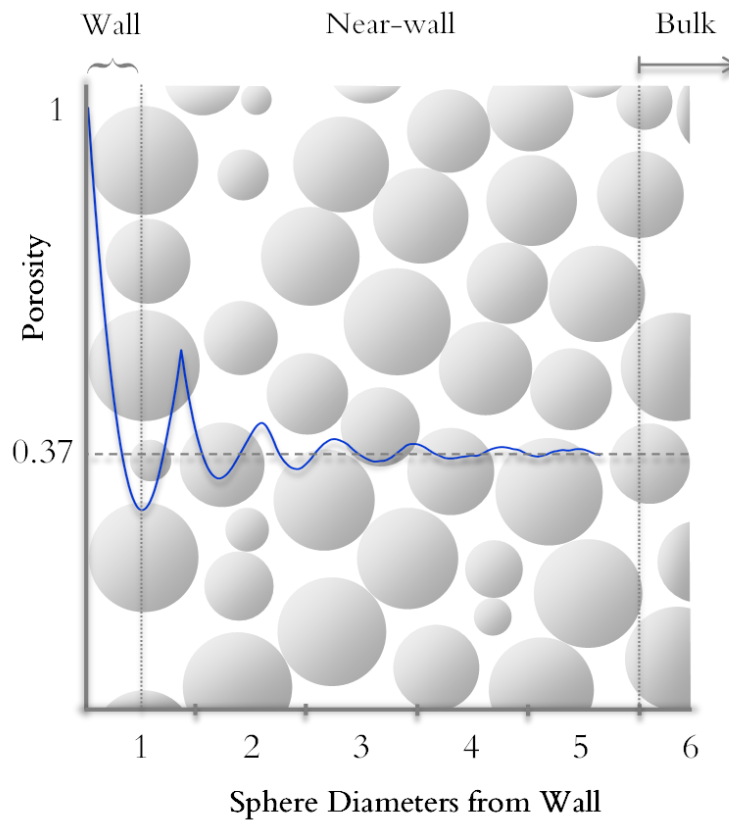


Figure 2.1: Porous structure in the wall and near-wall regions of an unstructured bed with average radial porosity overlain as a function of ball diameters with an average porosity of 0.37 in the bulk region.

The first, very prominent region, is referred to as the *wall* region and is located up to half a sphere diameter from the wall. The subsequent region, where the porosity is still oscillating greatly, is the *near-wall* region at between 0.5 and 3 to 5 sphere diameters from the wall. Finally, the region where the average porosity has more or less converged to that of the overall bed, is known as the *bulk* region.

For an annular bed, such as the HTTU experiment, the different observed regions are similar except that towards the inner wall of the annulus, the same oscillatory behaviour is apparent as towards the outer wall and therefore inner *near wall* and *wall* regions exist (Du Toit, 2008). This characteristic porosity distribution, along with the full analysis of the porosity of the HTTU, is described further in Chapter 3.

2.1.2. Application of DEM to generate packed beds

Discrete element method (DEM) modelling, as a Lagrangian approach to particle tracking, interaction and dynamics, is a suitable technique to generate a representative packed bed. By obtaining data of the geometry such as the porous structure, sphere centre points and contacts, the numerical description of the bed may be used directly in explicit flow and heat transfer models.

Using uniform spheres as particles in numerical DEM codes simplifies geometric constraints and interactions, thereby resulting in relatively fast computational times, especially when using graphical processing unit (GPU) solving. By applying realistic material properties and spreading or randomising the injection location of particles above the bed, the resulting bed geometry is close to that of a manually packed unstructured bed.

A further application of this technique is to then analyse the porosity of the numerical geometry, such as discretising the axial and radial directions and obtaining average porosity values for the respective increments, thereby obtaining a description of the porous structure. This in turn may also be applied in a porous medium approach instead of a discrete geometry. By choosing different increments a coarser resolution of the porous medium can be described or simply a bulk average over the entire geometry.

For this study, the commercial DEM code ESSS Rocky² (ESSS, 2022) was applied to generate a representative geometry of the HTTU. This technique and the results related to the analysis done for this study are described in Chapter 3. This is foundational to the further steps of modelling the geometry and solving the flow and heat transfer numerically. The remainder of this section focusses on the application of DEM to generate packed bed geometries as found in literature.

Studies focused on the generation of PBR packed beds

Mitchell & Polson (2007) utilised the commercial code PFC3D (Particle Flow Code) to evaluate the loads on the centre reflector of the PBMR annular core.

The buildup of graphite dust due to friction between fuel elements is of concern in PBR cores. As it is not practical to conduct full scale tests, for this reason Rycroft *et al.* (2013) made use of the DEM software LAMMPS (Large Atomic/Molecular Massively Parallel Simulator) to evaluate a full-scale core as well as comparison to scaled-down geometries to quantify the difference.

In an evaluation of different wall structure geometries, Li *et al.* (2015) applied the DEM solver embedded in the open-source software OpenFOAM to evaluate packed bed structure-wall interactions.

In a similar approach where a packed bed geometry is generated by filling a cylindrical space and allowing particles to settle, Zhao *et al.* (2015) applied a self-developed soft sphere model DEM solver as a viable solution to obtain a static packing and eventually a dynamically moving packing.

Zou *et al.* (2024) generated a representative bed of the TF-PBEC experimental pebble bed and the full HTR-PM core using GPU-DEM a self-developed DEM code utilising GPU solving. The purpose of the method was to solve a particle-scale heat transfer model validated with experimental data and the

² At the time of use, Rocky was owned by ESSS in Brazil. The software has since been purchased by Ansys and is referred to as Ansys Rocky.

porosity was not analysed in this study, instead the porosity as necessary for correlations such as that of Nusselt number, was determined using the method of Mueller (2012).

Studies on the analysis of the porous structure of PBR packed beds

The GPU-DEM code was also used to model dynamic pebble flow in the core of the HTR-PM (Zhang, *et al.*, 2024) after validation of the porosity distribution (Zou, *et al.*, 2023).

Chapter 3 of this study focusses entirely on the packing structure and analysis of the porosity of unstructured beds of uniform spheres, in particular applied to the HTTU annular bed. In Section 3.2.3 the available literature of studies on the analysis of the porous structure is summarised.

Here it is already important to note the higher porosity near the walls in cylindrical and annular packings due to a more structured packing, as was shown in Figure 2.1. It is therefore expected to see a maximum velocity in the lowest porosity regions of the bed and local porous pockets could affect flow and therefore convective heat dispersion.

2.1.3. Modelling porous structures

Coutelieris & Delgado (2012) discuss analytical solutions to cell models of porous media with single phase flow. Cell models consider a control volume consisting of a fluid cell containing a solid particle, arranged in a certain way such that an analytical solution exists for the geometry formed. The 2-dimensional methods presented are either sphere-in-cell, cylinder-in-cell or spheroid-in-cell approaches.

These cells could be considered also in 1-D or in 3-D, the latter approach leading to the possibility of studying porous structures using the Lattice Boltzmann method (LBM). Important transport phenomena present in porous structures include diffusion, axial dispersion, and radial dispersion.

Where the discrete flow domain is not modelled, a semi-analytical approach may therefore be taken to model the physical phenomena in the flow and solid domains using correlations. Later in this chapter, the semi-analytical and explicit numerical approaches to modelling in porous structures of PBRs, are discussed.

Auwerda *et al.* (2010a) considered the neutronic effect of simplifying a PBR core to a homogenous porosity, compared to using radial zones and discrete fuel elements. The result on the effective multiplication factor ($k_{eff,reactivity}$) for different packing fractions was investigated, and the effects compared to measurements done on the HTR-PROTEUS zero-power critical facility at the Paul Scherrer Institute in Switzerland. Similarly, Hao *et al.* (2022) performed an uncertainty analysis on the $k_{eff,reactivity}$ of the HTR-10

core due to random packing of fuel elements using a grid-based Expanding System Method (ESM) to generate an explicit bed.

2.1.4. Pebble Bed Hydraulics

The focus of this study is primarily on the modelling and validation of integral heat transfer effects in the HTTU and for this reason no in-depth discussion is made on the literature of flow and pressure drop through packed beds in particular, as several studies have done so in the past. Only the necessary details as pertinent to forced convective flow, as it is a significant component of the total heat transfer, will be addressed.

Flow behaviour

For the semi-analytical approach using a porous medium the inertial and viscous terms had to be implemented to characterise the pressure drop correctly and therefore a suitable correlation is discussed. The so-called wall channelling effect, shown in Figure 2.2, is accounted for with zones of different porosity, but local porous pockets are of course not resolved unless a discrete geometry is used.

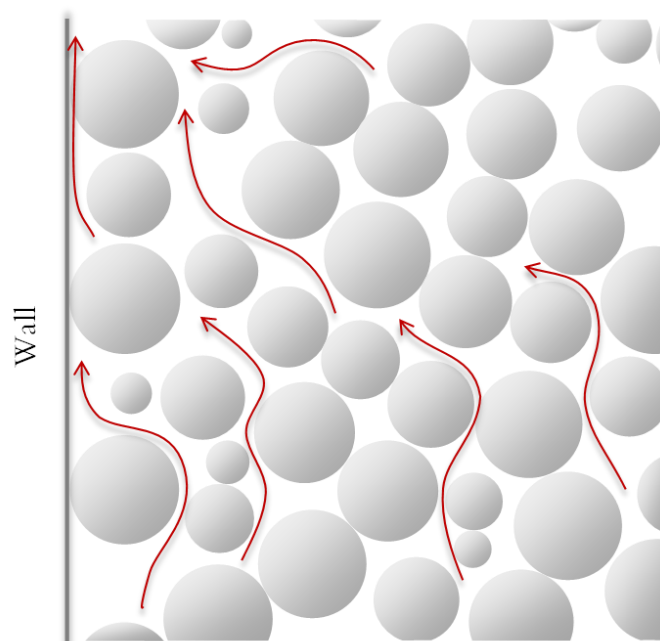


Figure 2.2: An illustration of the porous structure in a section of randomly arranged pebbles near the wall showing the channelling and braiding effect on gas flow.

Barker (1965) discusses that in general, the Colburn J-factor analogy needs to be adjusted for packed beds due to dispersion. This effect is discussed at the hand of examples from experimental work including spherical elements.

Velocity profile

Bey & Eigenberger (1997) remarked from experimental results that the velocity profile is important for the design of a fixed bed process in the chemical industry, including unstructured beds of uniform spheres. The maximum in the velocity profile was seen in the vicinity of walls and bypass-flow behaviour leads to inaccuracies if applying a correlation for a single effective porosity, in both flow and heat transfer predictions. Experimental work to characterise this bypass flow has been done by Amini & Hassan (2014).

It is clear that heat transfer at the wall would also be greatly affected (Daszkowski & Eigenberger, 1992) and for the HTTU where heat input is applied from the inner reflector it is a critical parameter to accurately account for.

In Chapter 5 the velocities measured above the bed of spheres in the HTTU, are presented. In the subsequent results section, the values calculated above the bed of spheres for the numerical cases are compared with the corresponding measurements for validation of the numerical flow fields.

Pressure drop

The Ergun equation (Ergun & Orning, 1949), (Ergun, 1952) as a correlation for pressure drop through a porous structure is widely applied in packed columns in the chemical industry, as evaluated by Daszkowski & Eigenberger (1992). The Ergun correlation for pressure drop over a packed bed of uniform spheres with diameter d_p and porosity ε of length L is given by:

$$\frac{\Delta p}{L} = \frac{150}{d_p^2} \cdot \frac{(1-\varepsilon)^2}{\varepsilon^3} \cdot \mu \cdot v_s + \frac{1.75}{d_p} \cdot \frac{(1-\varepsilon)}{\varepsilon^3} \cdot \rho \cdot v_s^2 \quad (2.1)$$

with μ the dynamic viscosity, ρ the density and v_s the superficial velocity of the fluid (calculated as if the geometry did not contain solids). The first term in Eq. (2.1) is the viscous and the second the inertial contribution to pressure drop. In CFD codes when defining a porous medium, the two terms are often defined separately in order to define the momentum conservation equation. Whilst the contribution of both terms is important when implementing a correlation of the Ergun-type, the inertial term becomes dominant for forced, turbulent flow in terms of the largest contribution to pressure drop.

Erdim *et al.* (2015) evaluated different pressure drop correlations for packed beds of uniform spheres at the hand of an experimental set-up. Considering all data points over different ranges of the Reynolds numbers and bed-to-particle-diameter ratios, the three correlations with the lowest calculated error values were found to be: i) the Darcy form of the friction factor obtained from linear regression from the particular experimental data in the study, ii) the correlation by Fahien & Schriver (1983) and iii) the correlation presented in the KTA standards (KTA, 1981).

The authors concluded that the oft-used Ergun pressure drop correlation is not suitable for packed beds of spheres with a modified Reynolds number above 500.

Du Toit *et al.* (2021) evaluated the friction factor correlations applicable to unstructured and structured packed beds consisting only of uniform spheres, including that of Erdim *et al.* (2015). In the latter, the authors reached a similar conclusion, that the Ergun correlation should be avoided in favour of that of the KTA (1981) and discussed the influence of the wall effect on the accuracy of the predicted pressure drop such that the use of the Einfeld & Schnitzlein (2001) correlation is best avoided for bed to particle diameter ratios below 2.

2.1.5. Heat transfer in Pebble Beds

The well-established experience of the Research Centre Jülich on the matter of pebble bed thermal-hydraulics is presented in Achenbach (1995). More recently, Almusafir *et al.* (2023) published a review of the phenomena and relevant correlations related to PBR thermal-hydraulics.

The porous structure of PBRs as has been described in this study gives rise to the typical flow behaviour in packed beds. Concerning heat transfer, the combination of fluid and solid domains mean that the physical phenomena usually associated with a solid material and in this case gas as fluid, would be present in each. Additionally, the interface between media and the close proximity of pebbles results in further observed effects, such as stagnant gas conduction as well as a greatly reduced reach of radiative heat transfer.

As illustrated in Figure 2.3, the different modes of heat transfer in an unstructured pebble bed could be classified as:

- Solid conduction through pebbles (**yellow**)
- Conduction through pebble contacts (**orange**)
- Stagnant gas conduction (**green**)
- Convective heat transfer to/from pebble surfaces to gas (**red**)
- Pebble-pebble and pebble-wall radiation (**purple**)

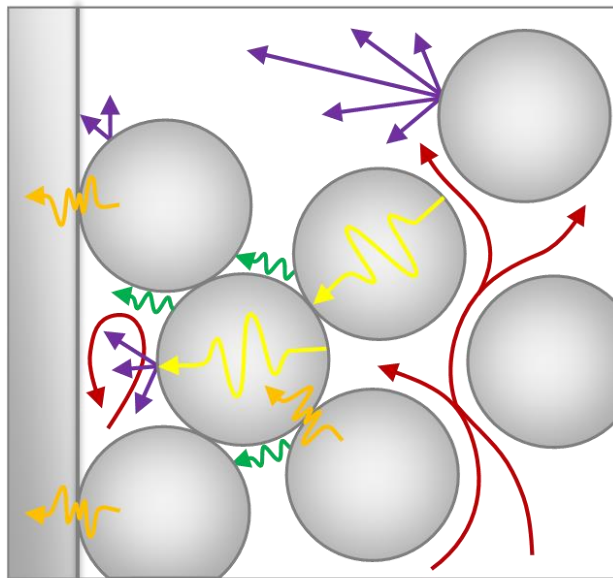


Figure 2.3: Different modes of heat transfer in an unstructured pebble bed.

A critical review was done on the published work of heat transfer in packed beds under forced convection of a gas in the chemical and petrochemical industry by Balakrishnan & Pei (1978) considering in their evaluation all the forms of heat transfer that need to be accounted for. Large discrepancies in the Nusselt number predicted by several authors was observed and the importance of experiments that consider similar conditions to that being modelled. None of the models mentioned were considered by other authors in the nuclear field such that their relevance cannot be evaluated here.

Effective thermal conductivity

In the porous media approach, the radiation heat transfer between the solids, the contact heat transfer between the solids, the conduction through the solids and the conduction through the stagnant gas are typically combined into an effective thermal conductivity (Van Antwerpen, 2009).

The earliest model to determine the effective thermal conductivity in a pebble bed found in literature is the Zehner-Schlünder (ZS) model (Zehner & Schlünder, 1970) which accounted for the conduction through two solid hemispheres in contact, as well as through stagnant gas in the small gaps.

Breitbach & Barthels (1980) improved upon the ZS model by including the contribution of thermal radiation. A further improvement on the model was made by Bauer & Schlünder (1978) to include the thermal contact resistance between spheres and this updated model is known as the Zehner-Bauer-Schlünder (ZBS) model. Both the ZS and ZBS models assume a uniform bulk porosity and thus do not explicitly take account of the different porous regions in an unstructured pebble bed.

Another correlation, that was developed from HTTU test data by Van Antwerpen (2009) to include the near-wall region, is the Multi-Sphere Unit Cell (MSUC) model. Aside from validation with the HTTU experiment, this model has also been evaluated against other correlations and for the set of SANA-I experiments (Van Antwerpen, *et al.*, 2012).

In a study by Wang *et al.* (2016), the authors propose a new theoretical model to determine the effective thermal conductivity and compare it to other models including ZBS and MSUC. This new model showed better agreement when compared with the results of an experiment by Robold (1982) of an unstructured bed of uniform steel spheres.

In their textbook on porous media, Vafai *et al.* (2005) put forth that the dispersion and tortuosity values in a porous approach may be calibrated from analysing a discrete geometry.

A remark is made that in a nuclear pebble bed core, different levels of irradiation of fuel spheres and surrounding material have an effect on the conductivity and ultimately create uncertainty in effective thermal conductivity.

Contact resistance

The contact resistance model developed by Bahrami, *et al.* (2005) and applied to an unstructured bed of rough spheres (Bahrami, *et al.*, 2006) was used as a basis by Van Antwerpen (2009) and De Beer (2021). With the Bahrami model as point of departure, the contact resistance model of De Beer (2021) was calibrated with data from the NWTCTF experiment (discussed in Section 2.2.2) as is used further in this study for the discrete geometry approach when defining contact resistances in the numerical model.

Radiation

Radiative heat transfer in dispersed or porous media is of importance to accurately predict temperatures and the effective thermal conductivity. Due to the high temperatures in PBR cores, the contribution from radiation plays a significant role in the overall heat transfer. A summary of the state of literature is provided in Howell, *et al.* (2021). Several models specific to PBRs have been suggested in literature to accurately model the contribution of radiative heat transfer.

In the study done by Pitso (2011) the author proposed a unique approach to characterising radiation heat transfer in randomly packed pebble beds. The Spherical Unit-cell Network (SUN) model uses a three-dimensional unit cell as the name suggests, consisting of several concentric spherical shells encasing a central sphere located in the bulk region and limiting the radiation emitted from the central volume to certain layers as is the case in an actual bed.

The MSUC model (Van Antwerpen, 2009) described previously did not initially describe the long-range radiation (radiation through the gaps between nearby spheres to more distant spheres) fully, which led to inaccuracies. Once the model included a component for the long-range radiation it showed good agreement with HTTU and SANA experiments.

Van der Walt (2020) described a so-called zonal-approach as adapted to beds of uniformly sized spheres. As a network-type approach this model divides the pebble bed geometry into different zones for more precise treatment of heat flux and temperature distribution. The results of this approach were compared with CFD and experimental results. Uncertainty of the contact resistances leads to an under-prediction of temperatures.

Convection

Although the NWU HTTU experiment did not generate heat within the pebbles, as is the case in a nuclear reactor, the literature with relevant correlations for the heat transfer in this case, is included due to relevance to the topic.

Hunt & Tien (1990) include analytical formulation for cases of reaction processes with sources of energy. For the chemical industry, this is relevant where multiphase and packed beds consisting of non-uniform particles need an analytical solution. For a bed of uniform particles with a known porosity distribution, the formulation may be simplified.

In the porous media approach, the modelling of the convection heat transfer between the spheres and the gas flowing through the packed bed must be accounted for. The required heat transfer coefficient is typically obtained from Nusselt number correlations.

Gunn (1987) proposed following correlation for the Nusselt number based on a comprehensive analytical and experimental analysis:

$$Nu = (7 - 10\varepsilon + 5\varepsilon^2)(1 + 0.7 Re^{0.2} Pr^{1/3}) + (1.33 - 2.4\varepsilon + 1.2\varepsilon^2) Re^{0.7} Pr^{1/3} \quad (2.2)$$

For $0.35 < \varepsilon < 1.0$ and form of the correlation satisfies the condition $(\partial Nu / \partial \varepsilon) = 0$ as $\varepsilon \rightarrow 1$.

Using an experimental set-up, Abdulmohsin & Al-Dahhan investigated the convective heat transfer (2015) and axial dispersion and mixing (2016) in an unstructured pebble bed made of glass marble spheres and found good agreement with the model of Gunn.

Gnielinski (1981), (2010) developed a semi-empirical method based on the assumption that the heat transfer from a particle to a fluid can be predicted by applying the equations for a flat plate by introducing a suitable length scale and a characteristic velocity. The asymptotic solution for the Nusselt number for laminar flow Nu_l is then:

$$Nu_l = 0.664 Pr^{1/3} (Re_p / \varepsilon)^{1/2} \quad (2.3)$$

Where $Re_p = \rho U_o d_p / \mu$ the Reynolds number and U_o the superficial velocity. The asymptotic solution for the Nusselt number for turbulent flow Nu_t is:

$$Nu_t = \frac{0.037 (Re_p / \varepsilon)^{0.8} Pr}{1 + 2.443 (Re_p / \varepsilon)^{-0.1} (Pr^{2/3} - 1)} \quad (2.4)$$

The combined solution of laminar and turbulent effects for flow over a single sphere is given by:

$$Nu_{sp} = 2 + \sqrt{Nu_l^2 + Nu_t^2} \quad (2.5)$$

Considering the shape factor for a bed consisting of spheres of equal size as is the case for the HTTU, the Nusselt correlation is then given by:

$$Nu = Nu_{sp} + 1.5(1 - \varepsilon) Nu_{sp} \quad (2.6)$$

The correlation is valid up to high Reynolds numbers, $0.26 < \varepsilon < 0.935$ and $0.7 \leq Pr \leq 10^4$.

The German safety standard KTA3102.2 (KTA, 1983) specifies that the Nusselt number for the heat transfer between the gas flowing through a pebble-bed and the pebbles shall be determined using the correlation:

$$Nu = 1.27 \frac{Pr^{1/3}}{\varepsilon^{1.18}} Re_p^{0.36} + 0.333 \frac{Pr^{1/2}}{\varepsilon^{1.07}} Re_p^{0.86} \quad (2.7)$$

The validity range of the correlation is given as $100 < Re_p < 105$, $0.36 < \varepsilon < 0.42$, $D/d_p > 20$ and $L_{bed} / d_p > 4$. D is the diameter of the bed and L_{bed} the length of the bed considered. If the local value for the porosity is used instead of the value averaged over the area, the restriction on D/d_p may be relaxed. In the case of unobstructed flow into the bed only half the value, based on the average porosity given by the correlation should be used for the pebbles forming the first layer. The expanded uncertainty for the Nusselt number is given as 20 % for a confidence level of 95 %.

2.2. Experimental Facilities

2.2.1. Integral Effects Tests

SANA (Forschungszentrum Jülich, Germany, 1994)

The *Selbsttätigen Nachwärmeabfuhr* (SANA) experiment (Lange, 1995) consisted of an unstructured annular bed of uniform spheres with a central heating element in order to investigate decay heat removal under natural convection. The facility was first operated from 1994 for two years during which data for several test configurations was generated, including spheres of two different diameters, nitrogen and helium gas atmospheres, as well as heat applied at different heights through the central heating element.

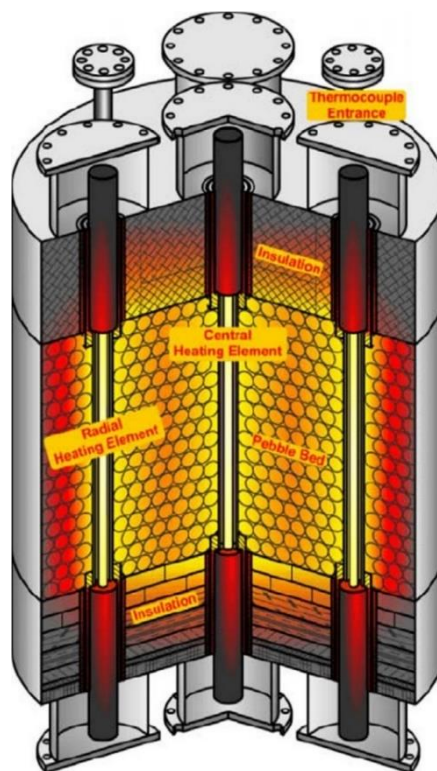


Figure 2.4: Section of the SANA experiment, showing all heater elements in full-height configuration (Stöcker & Nießen, 1997).

The data sets of the SANA experiment have been published by Stöcker & Nießen (1997) and have often been used to perform the validation of codes applied to conduction and radiation models for effective thermal conductivity evaluation and also for natural convection in decay heat removal. Studies that have relied on this data include the work by Becker & Laurien (2003), Du Toit *et al.* (2006), Lim & No (2006), Rousseau *et al.* (2006), and Novak *et al.* (2019). Forced flow convection tests were not performed in the SANA facility as it was not designed for this configuration.

HTTU (North-West University, South Africa, 2007)

As part of the qualification program of the PBMR, the Heat Transfer Test Facility (HTTF) (Rousseau & Van Staden, 2008) was constructed by PBMR (Pty) Ltd. in cooperation with the North-West University and M-Tech Industrial (Pty) Ltd. in South Africa, with the goal of furthering validation efforts of the flow and heat transfer phenomena in an unstructured annular pebble bed under similar operating conditions to that of the PBMR-400 design. The non-nuclear High Temperature Test Unit (HTTU) consisted of an annular bed with full-size 60 mm pebbles representative of the core of the PBMR-400 in terms of distance between reflectors but of a reduced height. The objectives of the facility were to determine the effective thermal conductivity (Rousseau, *et al.*, 2014), investigate natural convection decay heat removal as well as performance under forced convective flow conditions.



Figure 2.5: A photograph of the HTTU facility at the Potchefstroom Campus of the North-West University.

The full data sets of the HTTU have not been published, but the work of Van Antwerpen (2009) and Rousseau *et al.* (2014) provides context and comparison to test cases under near-vacuum radiation as well as nitrogen and helium atmosphere natural convection conditions. Data from the HTTU has been used in V&V efforts of models (Hoffmann & Janse van Rensburg, 2006).

An analysis of the axial, radial, and bulk porosity of a representative DEM model of the HTTU packed bed has been published previously (Potgieter & Du Toit, 2023) and is re-published here in its entirety in Chapter 3.

TF-PBEC and TF-PBF3D (INET, China, 2016)

In support of the HTR-PM project, the Institute of Nuclear and New Energy Technology (INET) at Tsinghua University in Beijing developed and operated several test facilities. As stated by Zhang *et al.* (2016) as the only published reference for the test facilities, the Test Facility – Pebble Bed Equivalent Conductivity (TF-PBEC) is described as a facility for the measurement of pebble bed effective thermal conductivity and the Test Facility – Pebble Flow 3D (TF-PBF3D) as a facility for the three-dimensional simulation test for pebble-bed flow.



Figure 2.6: The engineering lab for the HTR-PM at INET in China (Zhang, *et al.*, 2016).

Ren, *et al.* (2017) published an analysis of the effective thermal conductivity ($k_{eff,conductivity}$) using test data from the TF-PBEC heat transfer test facility, compared to a previous formulation using data from the SANA experiments.

2.2.2. Separate Effects Tests

HPTU (North-West University, South Africa, 2006)

Another facility at the NWU was the High Pressure Test Unit (HPTU) that focussed on the high pressure flow and thermal dispersion effects for the PBMR. The HPTU had several test bed sections, all of which were of a structured body-centred-cubic (BCC) packing however and is therefore not considered for this study. In the Braiding Effects Test Sections (BETS) the test sections had different homogenous porosities, ranging from 0.36 to 0.45 (Du Toit, *et al.*, 2014) which is provided as a reference relevant to the thermal dispersion in the different porous regions that should be accounted for in numerical models of an unstructured pebble bed. The facility was also used to determine the pressure drop over a structured bed (therefore fixed bulk porosity) for a range of Reynolds numbers (Du Toit & Rousseau, 2014).

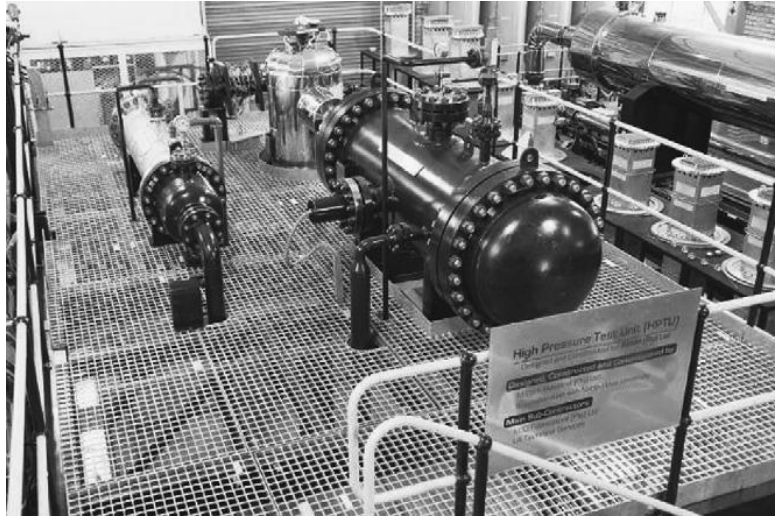


Figure 2.7: Photograph of the completed HTTF-HPTU facility (Rousseau & Van Staden, 2008).

PIV and RIM (Texas A&M University, 2007)

Using translucent spherical elements, Hassan & Dominguez-Ontiveros (2008) were able to perform visual measurements of the inter-pebble flow in certain gaps shapes using particle tracking velocimetry (PTV) in order to contribute to the calibration of CFD models.

NWTCTF (North-West University, South Africa, 2015)

The Near-Wall Thermal Conductivity Test Facility (NWTCTF) (De Beer, *et al.*, 2017) shown in Figure 2.8 was developed by the SARChI Chair in Nuclear Engineering at the North-West University in South Africa in order to investigate the near-wall effects on conduction and radiation of a structured and unstructured pebble bed at temperatures up to 1600 °C.

A comprehensive study summarises the published work, numerical method and both numerical and experimental results was published by (De Beer, 2021).

A calibrated expression for the pebble thermal contact resistance as determined by CFD modelling of the NWTCTF is included in the discrete geometry approach presented in this study (see Section 4.3.7).

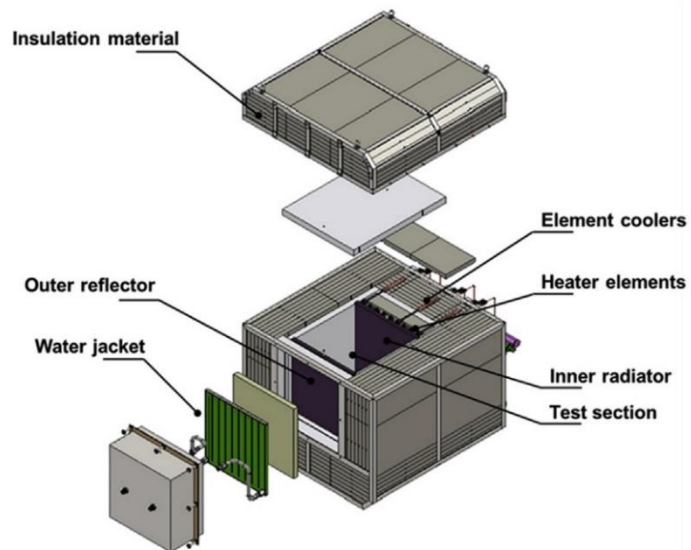


Figure 2.8: A photo of the NWTCTF vessel and internals (left) and exploded view of the test section components (right) from (De Beer, et al., 2018).

Experiment to measure mixing phenomena (Missouri University of Science and Technology, 2015)

Abdulmohsin & Al-Dahhan (2016) investigated the gas mixing in an experimental set-up of cylindrical bed consisting of glass spheres for different aspect ratios using cold air as fluid with a gaseous tracer gas. The resulting dispersive Peclet number as a function of modified Reynolds number was compared to other empirical correlations.

Small-scale experimental set-up (Handong Global University, South Korea, 2017)

In order to better investigate the local hot-spot effects of heated pebbles in a packed bed, a small face-centred-cubic (FCC) test section was developed at the Handong Global University (Chen & Lee, 2017) using a spherical heater element with a representative FCC geometry section of 14 faces in contact.



Figure 2.9: Top view of the test section from Chen & Lee (2017).

2.2.3. Nuclear Tests

HTR-10 (INET, China, 1995)

The HTR-10 experimental reactor at the INET of Tsinghua University in Beijing served as a scaled plant demonstrator for the planned HTR-PM (Xu, 2002). The reactor reached criticality in 1995 and was subsequently the subject of several safety demonstration experiments such as LOCA, control rod fault and turbine trip (Zhang & Yu, 2002). The facility also served as an integral test of a nuclear heated fuel pebble bed up to 1600 °C (IAEA, 2003).



Figure 2.10: The reactor and turbine buildings of the HTR-10 facility in Beijing, 2016 (author's own photograph, taken with permission).

2.2.4. Fuel Temperature Tests

AVR melt wires

Temperatures in prototype reactors are measured due to uncertainty in design calculations in order to verify obtained temperatures. In PBRs with online refuelling (hence a dynamic bed) this may be done by adding blank fuel elements with a series of melt wires consisting of alloys corresponding to a certain melting temperature. In the AVR this was done with a test pebble containing 20 wires and left to pass through the core of the reactor and it was observed that temperatures exceeded the expected values,

especially in the outer regions of the cylindrical core (Kugeler, *et al.*, 2017), reaching up to 1375 °C. An example of such a test pebble is shown in Figure 2.11 below.

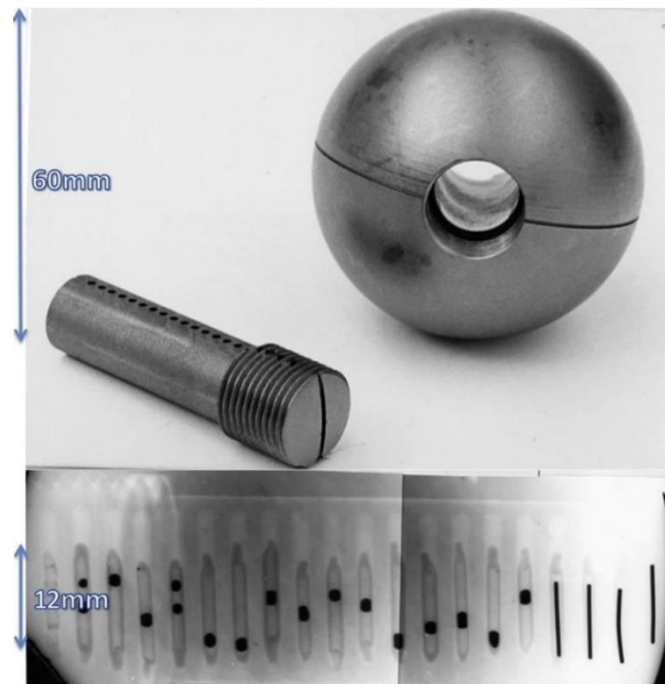


Figure 2.11: Blank test pebble (containing no fissile material) for temperature measurement by means of melting wires (top) and an x-ray of the insert after passing through the AVR (bottom) (Kugeler, et al., 2017).

2.2.5. Validation

Aside from the qualification of components, systems and technology, the purpose of test facilities is also to provide data for the validation of numerical codes to be used in design verification and safety analyses.

The validation of PBR codes or codes applied to the modelling of heated pebble beds is usually performed by using data from the SANA experiments (Stöcker & Nießen, 1997). Although numerous and covering ranges of power and location of heat source, nitrogen and helium as coolant, and different pebble size and materials, the experiment allows only for the validation of conduction and radiation models (for effective thermal conductivity) and natural convection circulation – in both cases only temperatures can be validated. Where validation has been done using the HTTU experiments (Rousseau & Van Staden, 2008) it was performed using similar cases, with models for effective thermal conductivity.

A main topic of this study is to validate CFD methods with data from the HTTU. The validation of different models in literature is discussed further in this Chapter, at the hand of the method and approach used.

2.3. Analytical Methods

2.3.1. KTA 3102

As a legacy from the licensing of pebble bed reactors in West Germany, the accepted Safety Standards of the KTA are for an analytical approach and remain as the only validated correlations pertaining to the thermal-hydraulic design of PBRs. Also translated into English, the relevant standards are:

- KTA 3102 Part 1: Calculation of the Material Properties of Helium (1978)
- KTA 3102 Part 2: Heat Transfer in Spherical Fuel Elements (1983)
- KTA 3102 Part 3: Loss of Pressure through Friction in Pebble Bed Cores (1981)
- KTA 3102 Part 4: Thermohydraulic Analytical Model (1984)



Figure 2.12: An example of the KTA standard document KTA 3102.2 in German (KTA, 1983).

For the calculation of the fluid properties of Helium, the standard (KTA, 1978) provides an exponential function for density as function of pressure and temperature, a constant value for specific heat, an exponential function for dynamic viscosity as function of temperature, and thermal conductivity as a function of temperature and pressure, along with the standard deviation function for each.

The Kugeler-Schulten (KS) correlation for Nusselt number is provided in the standard (KTA, 1983) as used in the calculation of the convective heat transfer coefficient from pebbles to coolant.

A correlation for the pressure losses over a certain length is provided in the standard (KTA, 1981) in a modified form of a Carman (1937) type correlation, similar to the more recent Ergun (1952) equation, as a function of the modified Reynolds number, bulk porosity and particle diameter.

In the standard (KTA, 1984), the equations of an analytical model of the mass, momentum and energy balance of the gas and solid phases are provided, including a function for the temperature distribution inside pebbles as well as for surface temperatures. The formulations include parameters to account for radiation through emissivity, solid conduction and surface convection. For solid conduction, the effective radial and axial thermal conductivities are required as input, which depends on the output of experiments to determine these as specific to the geometry.

Where the geometry and defining parameters of a bed do not exactly match those of an experiment, the predicted $k_{eff,conductivity}$ would not be suitable for generalisations. The formulation of the KS correlation contains terms for the radial and axial components of mass flow, again dependent on experimental measurements. It should also be noted that the formulation uses a bulk porosity and no distinction is made between different regions, the effect of local porosity variations would have an influence on both the local flow and actual heat transfer. As these models do not distinguish between different porous regions, application to an annular bed such as the HTTU could result in inaccurate velocity and temperature distribution predictions.

The limitations and shortcomings of the analytical methods described by the KTA have been shown by several authors, in particular concerning the predicted pressure losses and concerning contact resistances.

2.4. Numerical Approaches

Allelein & Verfondern (2018) stated that a major open technical issue of HTR development in Germany that requires more in-depth investigation is the simulation capabilities, for pebble flow as well as more reliable thermal-hydraulic modelling inside the core. Numerical methods, such as DEM and CFD and hardware capabilities have advanced significantly in the past decades and enabled much more detailed and complex simulation of PBR flow and heat transfer phenomena.

For this study the definition of a semi-analytical method is made to refer to the use of correlations or analytical relationships to solve certain flow or heat transfer parameters in a model or numerical code. In particular, for a CFD code this would consist of the geometry defined by the porosity in a porous medium, as opposed to discrete geometry of the flow and solid heat transfer domains.

2.4.1. 1D/2D System-level codes

System-level or systems codes are typically limited to 1D or 2D approximation of physical problems and tend to favour a representative rather than a discrete approach for modelling geometry. This makes such programs agile and not as computationally expensive as other codes with a discrete approach. For axi-symmetric problems, or problems that can easily be approximated such as flow in straight pipes, systems codes have a high degree of accuracy.

Rousseau *et al.* (2019) described the application of different CFD and systems-level codes applied to the design analysis and safety assessment of HTRs. In Figure 2.13 the V-model of the systems engineering process is shown at the hand of simulations of nuclear plant design.

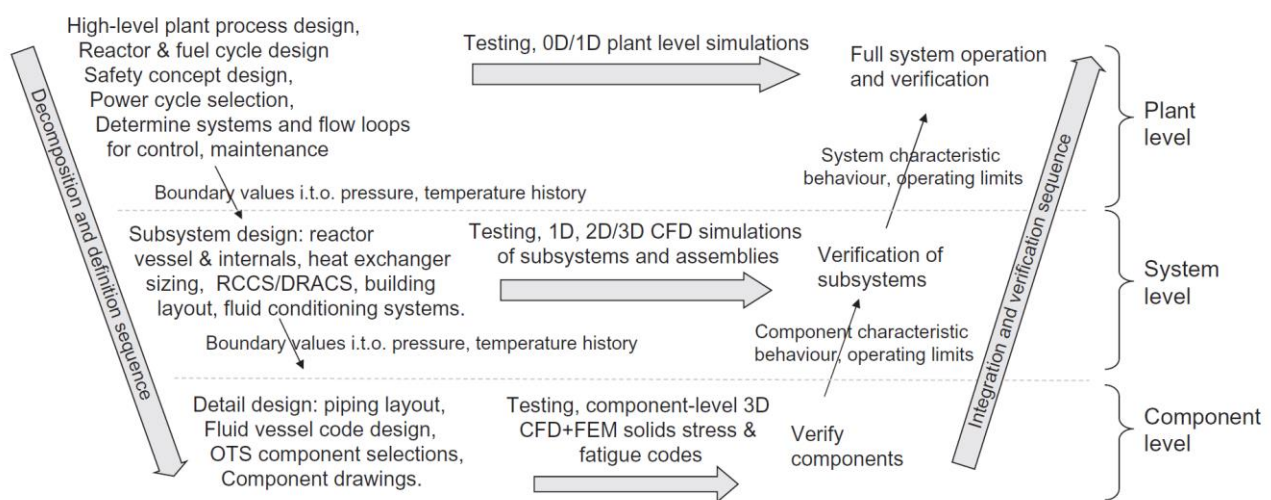


Figure 2.13: The V-model of the systems engineering process as it applies to nuclear power plant development (Rousseau, et al., 2019).

RELAP

The RELAP (Reactor Excursion and Leak Analysis Program) has been in development for several decades and is synonymous with the safety analysis of thermal-hydraulics of pressurised water reactors as well as other reactor technologies. With several branches of the code with different contributors and developers, one version namely RELAP5-MOD3 (Idaho National Engineering Laboratory, 1995) is often cited as applied in PBR analyses in the past.

Scari *et al.* (2016) applied RELAP5-3D to model the HTR-10 core and analysed the steady state and transient behaviour, comparing the numerical results to that with published benchmark data.

GAMMA+

The GAMMA+ (GAs Multicomponent Mixture Analysis plus) code was developed by the Korea Atomic Energy Research Institute (KAERI) as a transient multi-physics code for safety analyses (Jun, *et al.*, 2009) including point-kinetic neutronics as well as chemical interaction between oxygen and graphite. The code has been validated against experimental data from the SANA experiments (Lim & No, 2006) and compared to results from other codes such as TINTE and THERMIX. GAMMA+ has been applied to model the HTR-10 safety demonstration experiments benchmark (Jun, *et al.*, 2007). The results from this numerical model of a loss of helium flow without reactor scram (LOFC ATWS) scenario were reported by Jun *et al.* (2009).

Flownex SE

Flownex SE (M-Tech Industrial, 2024) is a 1D systems-CFD (sCFD) code implementing an Eulerian approach to model several PBR components and equipment. Originally developed for the mining and aerospace industries, the code known at the time as Flownet, was developed much further during the PBMR project to be applied to coupled neutronic thermal-hydraulic safety analyses of the PBMR-400. Flownex SE has been verified and validated using PBMR experimental data according to industry standards such as ISO 9001 and NQA-1.

The code utilises a 2D network model for pebble bed reactors, with the possibility to define different porosity values to different regions, and correlations to account for different components of heat transfer.

In a related study, the results from a Flownex SE model of the HTTU were compared with good agreement with the experimental data alongside that of a representative porous medium approach in 3D CFD (Potgieter & Du Toit, 2024).

2.4.2. 2D/3D Representative geometry codes

The following codes are capable of modelling a 2D or 3D geometry of a pebble bed through a representative geometry based on a porous medium approach.

THERMIX

Initially developed at the Jülich research centre, THERMIX (Wolf, *et al.*, 1990) is a 2D thermal-hydraulics design tool and contains the empirical formulas of the KTA standards embedded in the code. (Zheng, *et al.*, 2012) THERMIX has been chosen for the design verification and safety analyses of the HTR-PM (Chen & Han, 2021). The authors Gao & Shi (2002) detailed how the simulation platform HTRSIMU, which is based on THERMIX, was applied to perform transient analyses of the HTR-10 in design basis and beyond design basis accident scenarios. These analyses were approved by the Chinese nuclear safety administration authority.

TINTE

A benchmark of the coupled neutronics and thermal-hydraulics for different transient design basis accident analyses of the PBMR-400 core was published by the NEA (2013). The benchmark made use of the TINTE (Time Dependent Neutronics and Temperatures) code as well as VSOP99 (Very Superior Old Program version 99) to generate the neutronic cross-sections at equilibrium conditions. Finally, THERMIX was used to calculate temperature distributions.

Pronghorn

Pronghorn is a finite element method (FEM) coarse mesh thermal-hydraulics simulation code, intended to bridge the gap between low resolution sCFD and high resolution but computationally expensive CFD (Novak, *et al.*, 2018). The code is based on the MOOSE (Multiphysics Object-Oriented Simulation Environment) framework and has been validated with data from the SANA tests (Zou, *et al.*, 2018). The code is capable of using a representative porous medium approach for modelling of pebble bed geometry.

A detailed description of MOOSE, the finite element as well as physics formulation of Pronghorn and results from models of the SANA experiments and the PB-FHR was done in the PhD thesis of Novak (2020). In the study, the innovative approach of describing the problem of PBR modelling in three different length scales: reactor ("macro"), pebble ("meso") and TRISO fuel particle ("micro"), is made in order to better account for the difference in temporal and spatial scales through this distinction.

SAM

According to Zou *et al.* (Zou, *et al.*, 2024) SAM (System Analysis Module) is a systems-level code developed by ANL for the safety analysis of HTGRs. Although SAM has been validated with the prismatic block HTTF experiment, it may be applied to PBR cores using a porous medium approach.

In the study by Zou *et al.* the authors used SAM to model the HTTU near-vacuum test case and compared the explicit pebble temperatures obtained from the code with the experimental results.

2.4.3. 3D Explicit geometry codes

When discussing codes based on computational fluid dynamics, it is important to note the level to which turbulence is resolved, as this has a significant impact on the computational power required or, practically speaking, the size of the geometry that can be solved on available computer hardware. A direct numerical solution (DNS) as the name implies, solves the Navier-Stokes equations of fluid motion directly without modelling smaller eddies and is therefore the most expensive computationally.

Large eddy simulation (LES) resolves large-scale turbulence and is necessary where the flow and its turbulent structures are highly transient. Reynolds-averaged Navier-Stokes (RANS) refers to a formulation where time-averaging is applied to the conservation equations and wall-effects are modelled.

There are several wall treatments that could be applied in a RANS model, depending on the CFD code used. A further distinction is made here with low-resolution or coarse mesh RANS using a representative porous medium for pebble beds. The latter is the least computationally expensive.

In Figure 2.14 below, a diagram of a pyramidal structure is shown where the base and apex represent the size of geometry that can be modelled with the respective approaches. In this study, both the so-called explicit geometry approach and the porous approach utilise a RANS turbulence model.

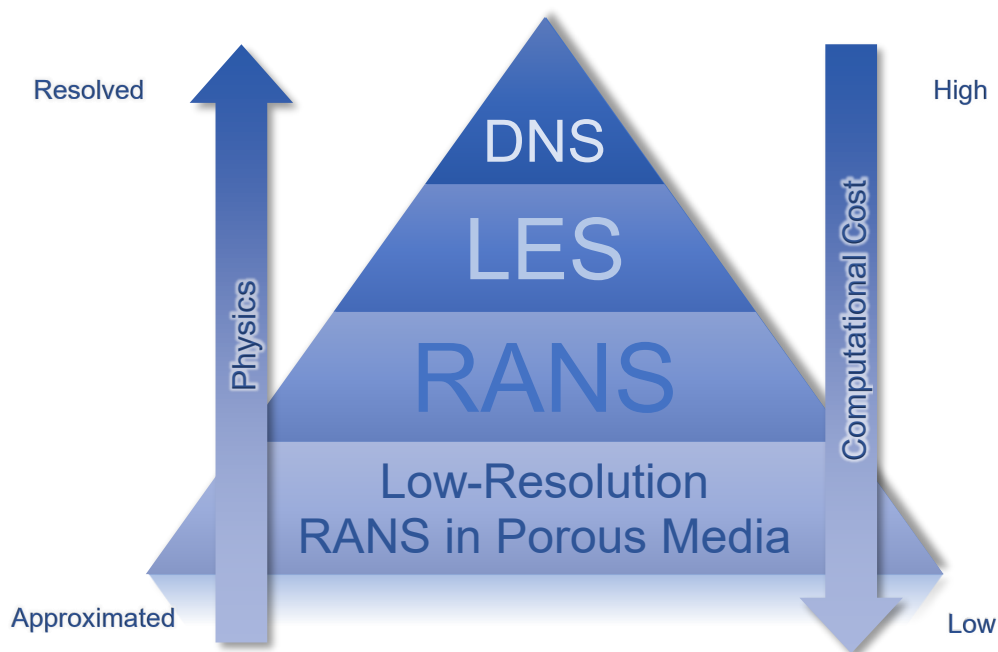


Figure 2.14: Approaches to Turbulence Modelling using Computational Fluid Dynamics

OpenFOAM

OpenFOAM (Open Field Operation And Manipulation) is a free and open-source CFD code (The OpenFOAM Foundation, 2024) offered under GNU GPL by several groups.

Auwerda (2014) developed a coupled code scheme to model the thermal-hydraulic and neutronic behaviour of pebble bed reactors. The thermal-hydraulic model was made in pebFoam (an OpenFOAM solver made for pebble bed geometry).

The PebBEx facility (Van Dijk, 2008) was used to measure the axial and radial porosity profile of a scaled-down cylindrical bed using a gamma-ray scanning technique (Auwerda, *et al.*, 2013). Combining this with the neutronic characteristics obtained from the zero-power critical test facility HTR-PROTEUS, the coupled simulation was applied to the HTR-PM reactor.

Dahl & Su (2017) published results from an OpenFOAM model of the HTR-PM using a porous medium approach.

Ansys Fluent

Fluent is a proprietary cell-centred CFD code (Ansys, Inc., 2024a) sold by ANSYS, Inc since 2006.

Jafari *et al.* (2008) modelled the flow in a cylindrical packed bed using the CFD software Ansys Fluent using a Reynolds-averaged stress model (RSM) and LES as turbulence models and evaluated the pressure drop and dispersion for a range of Reynolds numbers.

(Wu, *et al.*, 2010) compared the use of a porous media approach with a discrete geometry in Fluent. Whilst the porous approach was found to be much more computationally efficient (at fewer than 2 % of the cells compared to the discrete case) the authors remarked that it lacked detailed and localised effects, especially close to solid regions.

Peng & Sun (2016) investigated the thermal-hydraulics of the HTR-PM using Ansys Fluent with a porous media model and compared this to the results from THERMIX.

Ansys CFX

CFX, also acquired by Ansys, is an implicit CFD code (Ansys, Inc., 2024b) using a vertex-centred approach and is therefore limited to tetrahedral and hexahedral mesh topologies.

In the work of Hassan (2008), the author compared LES simulation in a section of pebble bed with measurements made using a particle tracking velocimetry (PTV) technique.

Yang *et al.* (2016) modelled pebble beds with low cylinder-to-particle diameter ratios with Ansys Fluent using RANS. The authors investigated the use of bridge contacts between spheres. This solution is further discussed in Section 2.4.5.

Siemens Star-CCM+

Star-CD and Star-CCM+ are proprietary CFD codes (Siemens, 2024) sold by Siemens PLM Software since 2016 after purchase of CD-Adapco.

Janse van Rensburg & Kleingeld (2011) described the integral approach to modelling the PBMR-400 reactor unit in Star-CD using RANS and a porous medium approach, including neutronic heat sources from fuel and irradiated materials.

Shams *et al.* (2014) performed an LES simulation of a section of randomly packed pebbles using Star-CCM+.

Van Staden *et al.* (2018) modelled a section of the Xe-100 PBR and riser tubes with Star-CCM+ using RANS and discrete pebble geometry with solid heat generation.

COMSOL

Weng *et al.* (2023) applied CFD with a discrete (particle-resolved) geometry to various packed bed catalytic reactor (in the chemical engineering industry) configurations, including spherical particle fill with air as fluid. The authors present a method to determine the heat transfer coefficient from particles to the fluid using CFD which is also applicable to CFD simulation of nuclear PBRs. The packed bed geometry in this study was generated with the 3D rendering software Blender and the CFD simulations were performed with COMSOL Multiphysics on a workstation with a relatively high amount of memory.

Nek5000 and NekRS

Nek5000 is a spectral element (SE) based open source CFD code (NEK, 2024) developed as part of the U.S. Department of Energy's Nuclear Energy Advanced Modelling and Simulation program (NEAMS). Fischer *et al.* (2022) expanded on Nek by including GPU solver libraries, making the code greatly scalable.

Reger *et al.* (2024) investigated the improvement of near-wall heat transfer in the porous medium approach of Pronghorn using a discrete pebble bed modelled with LES in NekRS.

2.4.4. Multiphysics and coupled codes

Coupled neutron-kinetics and thermal-hydraulics

Filippov *et al.* (2004) performed a full core analysis of a high power HTR design using a coupled neutronics and thermal hydraulics approach.

A 3D thermal-hydraulics code AGREE was coupled to a 3D spatial kinetics code PARCS by Seker & Downar (2007) to perform an analysis of the PBMR-400 benchmark (NEA, 2013). The AGREE model was also validated with data from the SANA experiments.

Venter and Mitchell (2007) described the design approach of the PBMR-400 which relied on models applied in an integrated way.

Suikkanen *et al.* (2014) developed a multi-physics system of codes to account for the intricate geometry and pebble interactions, neutronics and thermal-hydraulics using DEM, Monte-Carlo neutronics and CFD. The DEM code LIGGGHTS was used to obtain pebble coordinates sent to the Monte-Carlo neutronics code SERPENT and porosity and interfacial areas to the CFD code Ansys Fluent. SERPENT and Fluent were two-way coupled to transfer thermal power and temperature distribution.

Coupled DEM-CFD

In the field of nuclear engineering a coupled approach could be understood to mean a coupling of thermal-hydraulics and neutronics codes. With PBR designs with a continuous fuel cycle and dynamically moving bed, there is an application for the coupling of DEM and CFD codes.

In a study that integrates different numerical approaches (Wu, *et al.*, 2017), the authors applied DEM for the solid phase geometry and conduction which is mapped to CFD as a porous medium in which the flow as well as conduction and radiation heat transfer, is solved. The radiative heat transfer and thermal contact resistance between spheres are computed using Voronoi cells to calculate view factors as well as an effective thermal conductivity for the solid domain. The coupled model was validated against the low aspect ratio packed bed experiment reported on by Wen & Ding (2006) which was used to derive effective thermal conductivities and convective heat transfer coefficients under steady state and transient conditions. The specific software that was used is not mentioned in the study.

A coupled pebble-fluid interaction simulation was performed by Li & Ji (2013) using a self-developed CFD and DEM code for the fluid and particle phases, respectively.

In another coupled DEM-CFD study of a dynamic pebble bed (Tsory, *et al.*, 2013) the authors solved the gas and solid phases explicitly, accounting for particle-particle heat transfer to include contact and gas gap conduction, particle-wall heat transfer as well as fluid-particle heat transfer by means of models defined by user-defined functions in Ansys Fluent. Finally, the solid pebble temperature is updated through the DEM energy balance.

Most recently, Duchnowski and Brown (2024) published a review of the codes that have been used to model PBR multiphysics.

2.4.5. Contact point treatment in explicit 3D modelling

Modelling the flow domain between spheres in contact prove challenging for automatic meshing tools due to the small gap and high likelihood of cells in this location to have a high skewness. Dixon *et al.* (2013) investigated different solutions to contact point treatment in the flow domain. The authors discuss four possible modifications to the geometry to improve mesh generation near contact points between spheres: under-sizing the spheres thereby leaving *gaps*; oversizing spheres to create an *overlap*; extruding a cylinder with centreline perpendicular to the centres of each sphere to *bridge* the space; cutting away the volume that such a cylinder would occupy to *cap* both with a flat parallel gap. These proposed modifications are shown in Figure 2.15 below.

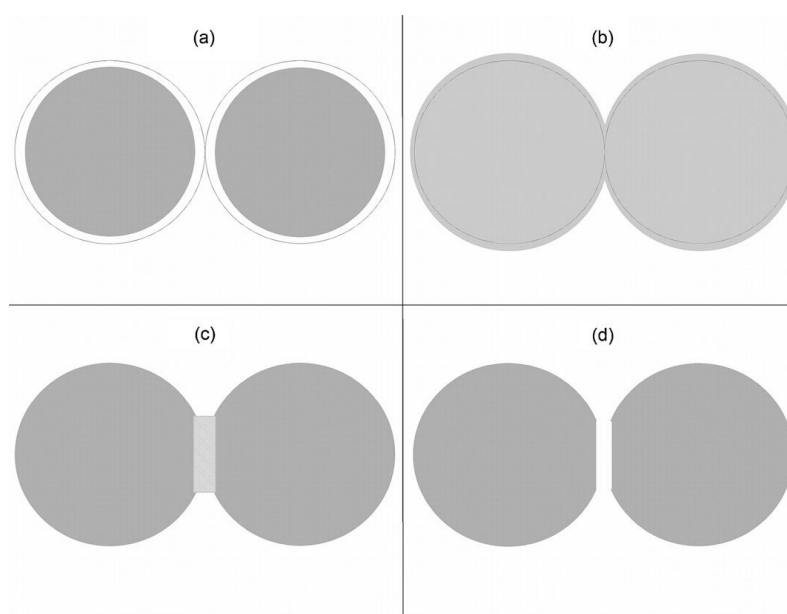


Figure 2.15: Drawing of four possible contact point modifications namely a) gaps, b) overlaps, c) bridges and d) caps proposed by Dixon *et al.* (2013).

Bu *et al.* (2014) applied the same methodology as above to structured packings of spheres that were simulated in CFX.

In a study by Lou *et al.* (2024) the authors developed a thermal resistance model for particle-particle contacts based on force for the localised heat transfer using DEM. The model was validated against the effective thermal conductivity tests done in the HTTU (Rousseau, *et al.*, 2014) with good agreement.

2.5. Contribution of This Work

This study focuses on both representative and explicit modelling of the forced isothermal flow, to build on the preliminary work that has been done by Reyneke (2009), and including forced convection that has not been before addressed to validate simultaneous radiation, conduction and convection and flow distribution modelling of the HTTU forced convection experiment.

2.6. Chapter Conclusions

It has been shown in this Chapter that, through the efforts of many authors, there are several suitable models and correlations that may be successfully utilised in finite volume CFD of packed beds and applied either to the discrete and fully resolved geometry or to a porous medium approximation.

The porous structure and by definition the porosity applied to models and correlations is the main source of uncertainty, as discussed where several models only using a bulk value are not entirely accurate, especially in the wall and near-wall regions.

The next Chapter is therefore dedicated to discussing the geometry and packing structure of the annular pebble bed of the HTTU in particular.

End of Chapter

✕

3. GEOMETRY AND PACKING STRUCTURE

Preamble

This chapter and its sections are based on the published work by the author from Potgieter & Du Toit (2023). The content of this chapter corresponds to the original source, except where some formatting changes or minor contextual corrections have been made in the text.

In this chapter, a comprehensive analysis of the porosity of the annular packed bed of the High Temperature Test Unit (HTTU) is presented. The annular packed bed is generated using a Discrete Element Method (DEM) approach. Semi-analytical methods are then used to analyse the porosity. The quality and representativity of the packed bed are established by evaluating the overlaps between spheres and spheres and walls and comparing the axial and radial variations in porosity with available experimental and numerical data. The angular and radial variation of selected sphere layers in the bottom near-wall region was studied revealing how the spheres in the axial layers and radial rings are staggered with respect to each other. The analysis of the radial variation in porosity also included the standard deviation and the skewness of the angular porosity at each radial position. An analysis of the radial porosity of the layers revealed that only first layer next to the bottom is markedly affected by the bottom wall. The interference between the oscillatory porosity variations perpendicular to the inner, outer, and bottom walls of the annular packed bed is demonstrated by the plot of the variation in porosity on an axi-symmetric r - z plane. The annular packed bed is also divided into 20 regions and the average porosity and the standard deviation of the porosity for each region is provided.

3.1. Chapter Introduction

Packed beds are prevalent in several industries, such as chemical processing and the food industry (Kolev, 2006) where applications are mainly focussed on separation and heat transfer processes. In the nuclear industry, several reactor designs have been based around a packed bed core design consisting of equal sized spheres (IAEA, 2013). The flow, pressure drop and heat transfer characteristics of a packed bed are dependent on the packing structure (Kugeler & Schulten, 1989); (KTA, 1983); (Rodríguez, *et al.*, 2021). The most influential characteristic of the porous structure is the porosity (Suikkanen, *et al.*, 2014); (Von Seckendorff, *et al.*, 2021). A proper understanding of the porosity and how it affects the phenomena that determine the performance of the packed bed reactor is therefore required (Novak, *et al.*, 2019).

Many physical experiments that were performed to determine the porosity of packed beds have been reported. Destructive approaches (Benenati & Brosilow, 1962); (Goodling, *et al.*, 1983) and non-

destructive approaches (Giese, *et al.*, 1998); (Guo, *et al.*, 2017) have been employed to determine the porosity directly. Imaging methods have also been widely used to determine the porosity. The most notable are X-ray radiography (Mueller, 1992), X-ray computed tomography (Reimann, *et al.*, 2017); (Von Seckendorff, *et al.*, 2021), gamma ray computed tomography (Auwerda, *et al.*, 2010b); (Al Falahi & Al-Dahhan, 2016); and magnetic resonance imaging (Sederman, *et al.*, 2001). The variation in porosity was either determined directly from the images (Reimann, *et al.*, 2017); (Al Falahi & Al-Dahhan, 2016); (Sederman, *et al.*, 2001), or else the coordinates of the centres of the spheres (Mueller, 1992); (Reimann, *et al.*, 2017); (Von Seckendorff, *et al.*, 2021) were determined by analysing the images. Packing algorithms (Mueller, 2005); (Jerier, *et al.*, 2010) and DEM (Theuerkauf, *et al.*, 2006); (Suikkanen, *et al.*, 2014) have been used to generate packed beds numerically. The coordinates of the sphere centre points can be obtained directly from these methods. The variation in porosity can then be calculated numerically using volume-based methodologies (Lamarche & Leroy, 1990); (Govindarao, *et al.*, 1990); (Mueller, 1992), area-based methods (Mariani, *et al.*, 2000); (Du Toit, 2002), (2019b); (Mueller, 2010), and line-based methods (Mueller, 2012); (Feng, *et al.*, 2021); (Bester & Du Toit, 2022).

Analysis of the experimental and the numerical data have shown that there is a marked influence on the packing structure exercised by the wall and the ratio between the cylinder diameter and the sphere diameter, or aspect ratio. It was observed that the porosity varies in a damped oscillatory manner from a value of one at the wall to a bulk value some distance from the wall depending on the aspect ratio (Benenati & Brosilow, 1962); (Goodling, *et al.*, 1983); (Giese, *et al.*, 1998). Empirical correlations having an exponential variation, such as by Vortmeyer & Schuster (1983), White & Tien (1987) and Hunt & Tien (1990), and having an oscillatory variation, such as by Martin (1978), Cohen & Metzner (1981), Mueller (1992) and De Klerk (2003), have been derived from and validated by the data. A selection of exponential and oscillatory correlations is evaluated by Von Seckendorff & Hinrichsen (2021). Du Toit (2008), Reyneke & Du Toit (2010) and Van Antwerpen *et al.* (2010) all assumed that in the case of an annular packed bed with the annulus width to sphere diameter ratio larger than ten, the empirical correlations may be applied to both the inner and the outer walls to obtain the variation in porosity in the direction perpendicular to each wall.

In order develop a better understanding of the porosity variations in annular packed beds, Du Toit (2008) compared the radial variation in porosity predicted numerically by several published correlations to firstly the porosity measured in experimental data and secondly to the porosity determined from the analysis of simulated packed beds, which were generated numerically by means of DEM. The packed beds considered were the HTTF (experimental and numerical) and the AP-HTTF (numerical) packed beds.

Reyneke & Du Toit (2010) considered the results of modelling the superficial velocity distribution inside an annular packed bed using Computational Fluid Dynamics (CFD) and a porous medium approach by

applying the different porosities of the AP-HTTF bed to sub-regions in the computational grid corresponding to regions in the bed with large porosity variations. They also obtained the local porosity from the weighted average of the porosity values associated with the inner, outer, and bottom walls based on the correlation of Martin (1978). It was shown that the porosity has a direct proportionate influence on the velocity distribution.

Reimann *et al.* (2017) and Du Toit (2019a) divided annular packed beds into radial and axial regions and calculated the average porosity for each region. Du Toit (2019a) also calculated the axial variation in porosity for the full cross-section of the AP-HTTF annular packed bed, as well for the inner and outer wall regions. Du Toit (2019a) concluded that the regional variation in porosity should be accounted for along with the radial variation in porosity when simulating the thermal-hydraulics performance of an annular packed bed.

A numerical model of the PBMR-400 annular packed bed was generated by Suikkanen *et al.* (2014) using a DEM approach. The radial variation in porosity of the bed generated was determined by using a methodology based on the experimental approach followed by Goodling *et al.* (1983). Suikkanen *et al.* (2014) found the results obtained to be in good agreement with the experimental data from Du Toit (2008). Suikkanen *et al.* (2014) also constructed a Voronoi cell around each sphere in the annular packed bed and calculated the porosity associated with each Voronoi cell. The results were then used to obtain the angular variation in porosity for selected cylindrical shells.

The method in this Chapter can be regarded as an extension of the work by Du Toit (2008), Reyneke & Du Toit (2010) and Du Toit (2019a) and endeavours to provide a more comprehensive evaluation of the HTTU annular packed bed (Rousseau & Van Staden, 2008). However, instead of analysing the AP-HTTU annular packed bed (Du Toit, 2008), a new numerical model of the HTTU annular packed bed was generated using the DEM code *ESSS Rocky*, version 4.3 (ESSS, 2022).

As a first step the quality and representativity of the HTTU model were evaluated. Secondly the angular and the radial variations in the porosity of the bottom wall and near-wall regions were considered to evaluate the influence of the axial variation in porosity. In the third step the interference between the radial variations in porosity from the inner and outer walls and the axial variation in porosity from the bottom wall was investigated by considering the variation in porosity on an axi-symmetric r - z plane. Finally, the HTTU annular packed bed was divided axially and radially into 20 regions of which the average regional porosities and standard deviations of the porosity were determined. The results can be implemented in a porous media CFD model to account for the effect of the variation in porosity on the flow and heat transfer.

3.2. Theoretical Background

3.2.1. Geometry of the HTTU annular packed bed

The Heat Transfer Test Facility (HTTF) was built by PBMR in order to investigate several physical phenomena associated with the PBMR-400 design, including the heat transfer phenomena in a packed pebble bed at high temperatures under forced and natural convection (Rousseau & Van Staden, 2008). Integrated effects tests could be performed on the experimental packed bed of the High Temperature Test Unit (HTTU) as constructed in this facility.

The HTTU was non-nuclear and consisted of an annular packed bed of spheres. At the inner radius the packed bed was contained by a graphite reflector with electrical heaters imbedded in it. At the outer radius the packed bed was contained by a graphite reflector surrounded by a water jacket to provide cooling. The geometry of the packed bed was representative of the annular core of the PBMR-400 (Rousseau & Van Staden, 2008) scaled such that it had a smaller inner diameter, but the same annular width, and only accounted for a part of its height as shown in Figure 3.1. The graphite spheres used were identical in size to the 60 mm pebble design which was to be used in the reactor. The annular packed bed was conceptualised to have an outer diameter of 2300 mm, inner diameter of 600 mm and total height of 1200 mm with flow entering from the heavily insulated bottom of the bed (Rousseau & Van Staden, 2008). The final outer diameter of the packed bed obtained from the design drawings was 2288 mm.

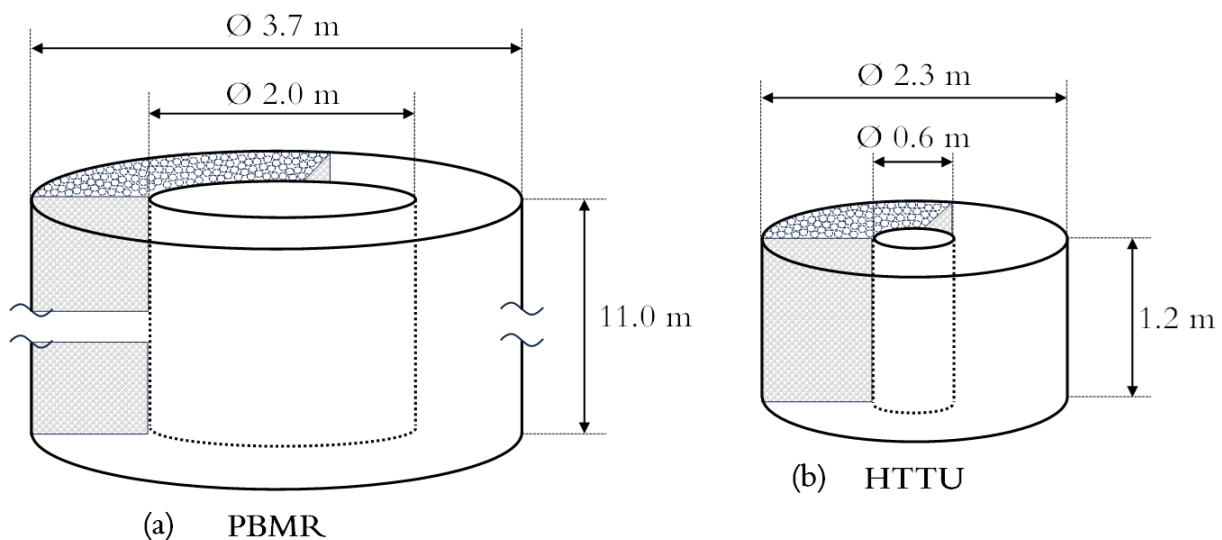


Figure 3.1: The geometry of the annular PBMR core (a), left and HTTU experimental bed (b), right.

With a larger outer to inner diameter ratio, the transition from wall to near-wall to bulk regions in the HTTU packing could be investigated to understand the operating conditions in the PBMR core (Rousseau, *et al.*, 2014).

3.2.2. Discrete Element Method (DEM)

The HTTU packed bed analysed in the study was generated numerically employing DEM. In DEM particles are described mathematically using a Lagrangian framework. This DEM approach models the particle kinematics in a discrete way with the equations of motion of particles derived from Newton's First Law as:

$$m \frac{dv}{dt} = F_g + F_c + F_{nc} \quad (3.1)$$

for translational movement, where v is the translational velocity, m the mass of a particle and the resultant force F due to gravitation (g), contact (c) and non-contact forces (nc), respectively.

Similarly, for rotational movement:

$$I \frac{d\omega}{dt} = \tau \quad (3.2)$$

where I is the moment of inertia, ω the angular velocity and τ the resultant contact torque acting on the particle.

The Figure 3.2 shows (a) two contacting spheres with overlap δ_N due to the normal contact force F_N and normal vector $\hat{n}$ and (b) two contacting spheres with tangential overlap δ_S and tangential force F_S in the direction of the tangential vector $\hat{s}$. The sum of contact and non-contact forces between interacting particles can also include adhesion force and rolling resistance models.

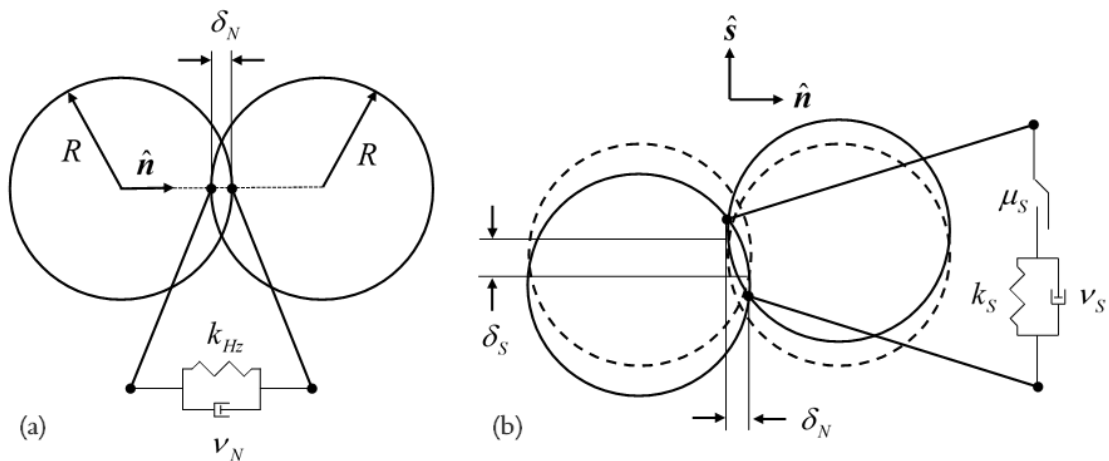


Figure 3.2: The contact between two equal sized spheres in the normal (a) and tangential (b) directions (sliding friction).

A soft-particle model of forces is commonly used in commercial numerical codes for DEM simulations and the treatment of normal and tangential forces have different models for linear or non-linear treatment of their coefficients.

This study produced numerically generated packed beds of equal sized spheres using the commercial DEM code *ESSS Rocky*, version 4.3 (ESSS, 2022). The specific models employed are the Hertzian spring-dashpot model for normal forces and the Mindlin-Deresiewicz tangential force model. The Hertzian spring-dashpot (or Damped Hertzian Spring) model treats the elastic and dampening components of the normal force as a non-linear function of the overlap (ESSS, 2022). The tangential force model of Mindlin-Deresiewicz treats the tangential stiffness as non-linear and hysteretic (Mindlin & Deresiewicz, 1953).

The damped Hertzian spring model of the normal contact force is described as:

$$\mathbf{F}_N = \left(-k_{Hz} \delta_N^{\frac{3}{2}} + c_N \dot{\delta}_N \right) \hat{\mathbf{n}} \quad (3.3)$$

where k_{Hz} is the Hertzian spring stiffness coefficient and c_N the damping coefficient. $\dot{\delta}_N$ is the derivative of displacement with respect to time – the relative velocity between spheres in the normal direction.

The stiffness coefficient is defined as:

$$k_{Hz} = \frac{4}{3} E \sqrt{R} \quad (3.4)$$

with E the Young's modulus of the spheres and R the sphere radii (Wassgren & Sarkar, 2008). The formulation presented here assumes the spheres are of uniform size and made from the same homogenous material.

For the model using a linear damped spring in series with a sliding friction element, the tangential force is given by:

$$\mathbf{F}_S = \min \left(k_S \delta_S + c_S \dot{\delta}_S, \mu_S |\mathbf{F}_N| \right) \hat{\mathbf{s}} \quad (3.5)$$

where μ_S is the sliding friction coefficient, k_S and c_S are the damped spring stiffness and damping coefficients in the tangential direction, respectively.

For the formulation by Mindlin & Deresiewicz (1953) the equation becomes:

$$\mathbf{F}_S = -\mu F_N \left(1 - \varsigma^{\frac{3}{2}} \right) \frac{\delta_S}{|\delta_S|} \hat{\mathbf{s}} + \eta_S \sqrt{\frac{6\mu^* F_N}{\delta_{S,\max}}} \varsigma^{\frac{1}{4}} \dot{\delta}_S \hat{\mathbf{s}} \quad (3.6)$$

With

$$\varsigma = 1 - \frac{\min(|\delta_S|, \delta_{S,\max})}{\delta_{S,\max}} \quad (3.7)$$

In the above equation η_s is the tangential damping ratio. The maximum relative tangential displacement $\delta_{s,max}$ occurs before the spheres begin to slide.

The approach implemented in *ESSS Rocky*, version 4.3 approximates the ratio as:

$$\eta_s = -\frac{\ln e}{\sqrt{\ln^2 e + \pi^2}} \quad (3.8)$$

with e the restitution coefficient of the sphere material.

The effective mass m^* is defined as:

$$\frac{1}{m^*} = \begin{cases} \frac{1}{m_1} + \frac{1}{m_2} & \text{for sphere-sphere contact} \\ \frac{1}{m} & \text{for sphere-wall contact} \end{cases} \quad (3.9)$$

The simulated packed beds were generated by spheres seeded from the top of the bed at a feed rate of 216 000 spheres per hour for a period of 500 s and were allowed to fall and roll into position in a natural way and was not compacted artificially. Therefore, only the weight of accumulating particles influenced changes in the packing structure over time as spheres were added. The simulation was continued for an additional 20 s to allow the spheres to settle. The final packed bed consisted of 30 002 spheres. The static and dynamic friction coefficients between spheres were taken to be 0.7 and the restitution coefficient of the spheres to be 0.3. The static and dynamic friction coefficient between spheres and walls were taken to be 0.3 and the restitution coefficient of the wall to be 0.3. The values used are in accordance with the values given by Luo *et al.* (2010) and used by Suikkanen *et al.* (2014) and Bester *et al.* (2021)

3.2.3. Methodologies to analyse porosity variation

This study employed the semi-analytical and numerical methods developed by Du Toit (2019b) and Bester & Du Toit (2022) to determine the porosity of the HTTU annular packed bed as consisting of equal sized spheres. The methods require that the sphere centre coordinates and diameter be known.

3.2.3.1. Axial variation in porosity

The cross sectional averaged axial variation in porosity $\varepsilon(z)$ for an annulus is given as (Du Toit, 2019b):

$$\varepsilon(z) = 1 - \frac{\sum A_i(z)}{\pi(R_o^2 - R_i^2)} \quad (3.10)$$

Where $A_i(z)$ the area of the intersection between the plane at level z and sphere i , R_o the outer radius of the annulus and R_i the inner radius of the annulus. The area $A_i(z)$ of the intersection is determined using analytical geometry (Du Toit, 2019b).

3.2.3.2. Radial variation in porosity

The radial variation in porosity is determined using a vertical line-based approach (Feng, *et al.*, 2021); (Bester & Du Toit, 2022). The porosity $\varepsilon(r_i, \theta_i)$ at radial position r_i and angular position θ_i between lower and upper axial limits z_l and z_h is given as:

$$\varepsilon(r_i, \theta_i) = 1 - \frac{\sum l_{ij}}{z_h - z_l} \quad (3.11)$$

Where l_{ij} is the length of the intersection between the line at position i and the sphere j accounting for the lower and upper limits. The tangentially averaged porosity $\varepsilon(r)$ at the radial position r can then be obtained from:

$$\varepsilon(r) = \frac{\int_0^{2\pi} \varepsilon(r, \theta) d\theta}{2\pi} \quad (3.12)$$

In this study the integrals are integrated numerically employing Simpson's Rule (Kreyszig, 2006). The standard deviation $\sigma_\varepsilon(r)$ of the tangentially averaged porosity at the radial position r is given as (Kreyszig, 2006):

$$\sigma_\varepsilon(r) = \sqrt{\frac{\sum_{i=1}^n \varepsilon^2(r, \theta_i) - 2\varepsilon(r) \sum_{i=1}^n \varepsilon(r, \theta_i) + n\varepsilon^2(r)}{n-1}} \quad (3.13)$$

Where n is the number of angular positions considered. The skewness $\mu(r)$ of the tangential variation of the porosity at the radial position can be obtained from (Kreyszig, 2006):

$$\mu(r) = \frac{\sum_{i=1}^n [\varepsilon(r, \theta_i) - \varepsilon(r)]^3}{(n-1)\sigma^3(r)} \quad (3.14)$$

De Klerk (2003) proposed two correlations that can be used to calculate or predict the radial variation in porosity when the coordinates of the centres of the spheres are not available. In a study of similar correlations Van Antwerpen *et al.* (2010) found the correlations of De Klerk (2003) to be the most suitable correlations to predict the radial variation in porosity for the HTTU annular packed bed.

The first correlation accounts for the radial variation in porosity for the approximately first half sphere diameter next to the wall, i.e. the wall region, and is given as:

$$\varepsilon(r) = 2.14(y^*)^2 - 2.53y^* + 1.0 \quad \text{for } y^* \leq 0.637 \quad (3.15)$$

Where y^* is the distance in sphere diameters from the wall. The radial variation in porosity for the near-wall and bulk regions is expressed as:

$$\varepsilon(r) = \varepsilon_b + 0.29 \exp(-0.6y^*) \cdot \cos[2.3\pi(y^* - 0.16)] + 0.15 \exp(-0.9y^*) \quad \text{for } y^* > 0.637 \quad (3.16)$$

In the case of the inner wall of the annulus we have that $y^* = (r - R_i)/d_p$ and for the outer wall $y^* = (R_o - r)/d_p$ where R_i and R_o are the inner and outer radii of the annulus respectively. In the case of the bottom wall y^* is replaced by $z^* = z/d_p$ to obtain $\varepsilon(z)$, the axial variation in porosity in bottom wall and near-wall regions.

3.2.3.3. Average porosity of a wedge

The average porosity $\bar{\varepsilon}$ of a wedge defined by the radial limits $r_1 \leq r \leq r_2$, angular limits $\theta_1 \leq \theta \leq \theta_2$ and the axial limits $z_l \leq z \leq z_h$, as described by Bester & Du Toit (2022), can be obtained from:

$$\bar{\varepsilon} = \frac{2 \int_{r_1}^{r_2} \left(\int_{\theta_1}^{\theta_2} \varepsilon(r, \theta) d\theta \right) r dr}{(\theta_2 - \theta_1)(r_2^2 - r_1^2)} \quad (3.17)$$

The evaluation of $\bar{\varepsilon}$ is performed first calculating the radial porosity $\varepsilon(r_i)$ at each radial position and then the average porosity by integrating the resulting radial porosity variation. The standard deviation $\bar{\sigma}_\varepsilon$ of the wedge porosity is given as:

$$\bar{\sigma}_\varepsilon = \sqrt{\frac{\sum_{i=1}^{n \times m} \varepsilon^2(r_i, \theta_i) - 2\bar{\varepsilon} \sum_{i=1}^{n \times m} \varepsilon(r_i, \theta_i) + (n \times m) \bar{\varepsilon}^2}{n \times m - 1}} \quad (3.18)$$

where m is the number of radial positions considered.

3.2.3.4. Axi-symmetric variation of porosity

The variation of the porosity $\varepsilon(r, z)$ in the axi-symmetric (tangentially averaged) r - z plane can be obtained by employing the tangentially averaged horizontal line-based method developed by Mueller (2012) and Du Toit (2019b) given as:

$$\varepsilon(r, z) = 1 - \frac{\sum S_i(r, z)}{2\pi r} \quad (3.19)$$

Where $S_i(r, z)$ is the length of the in-plane arc of the intersection between the cylindrical plane at radius r and the circular cut through sphere i at the level z . The length of the arc is determined using analytical geometry (Du Toit, 2019b). By defining a grid of (r, z) points between the limits $r_1 \leq r \leq r_2$ and $z_1 \leq z \leq z_2$ the variation of the porosity over the plane can be obtained.

3.3. Results

3.3.1. Evaluation of data

The first step in the analysis of the numerically generated HTTU annular packed bed model is to evaluate the quality and the representativity of the data. For this purpose, three additional annular packed bed models with Young's modulus values of $E = 0.01$ GPa, $E = 0.1$ GPa and $E = 1.0$ GPa respectively were generated along with the HTTU annular packed bed model with a Young's modulus of $E = 11.7$ GPa using the commercial DEM code *ESSS Rocky* (ESSS, 2022). The calculated overlaps between adjacent spheres, the spheres next to a wall and the wall, the maximum overlap, average overlap, number of overlaps, bulk porosity of the packed bed and the number of spheres in the packed bed are summarised in Table 3.1. Also included in Table 3.1 are the corresponding results for the AP-HTTF numerical annular packed bed model analysed by Du Toit (2008). The bulk region of the annular packed bed was taken as the part of the packed bed which is more than five sphere diameters from inner and outer walls and the bottom (Goodling, *et al.*, 1983), and below 1.2 m from the bottom. In DEM simulations the value of Young's modulus is typically decreased to reduce the computational cost (Yang, *et al.*, 2014).

It can be seen in Table 3.1 that the total number of overlaps and the maximum and average overlaps decrease as the value of the Young's modulus for the spheres increase. It can also be seen that the value of the bulk porosity for the packed bed with a Young's modulus of $E = 0.01$ GPa is markedly lower than the corresponding values for the other packed beds. Comparing the corresponding average overlap values for the HTTU ($E = 11.7$ GPa) and the AP-HTTF packed beds it can be seen in Table 3.1 that in the case of the sphere-sphere overlaps there is very good correspondence, but in the case of the sphere-wall overlaps those for the HTTU packed bed is larger. However, the number of overlaps per sphere is in the case of the HTTU packed bed is 25 % less than the overlaps per sphere in the case of the AP-HTTF packed bed.

Table 3.1: Summary of overlaps (OL) between spheres and between spheres and walls for the HTTU and AP-HTTF models.

Overlaps	$E = 0.01 \text{ GPa}$		$E = 0.1 \text{ GPa}$		$E = 1.0 \text{ GPa}$		$E = 11.7 \text{ GPa}$		AP-HTTF	
	spheres	walls	spheres	walls	spheres	walls	spheres	walls	spheres	walls
$0 \% < \text{OL} \leq 0.1\%$	1936	129	12295	135	44278	143	59929	57	112440	4200
$0.1 \% < \text{OL} \leq 1 \%$	47826	885	54641	618	22479	482	588	522	22	0
$1 \% < \text{OL} \leq 2 \%$	34905	398	3722	217	1	78	0	43	0	0
$2 \% < \text{OL} \leq 3 \%$	6053	10	319	1	0	0	0	0	0	0
$3 \% < \text{OL} \leq 4 \%$	310	0	31	0	0	0	0	0	0	0
$4 \% < \text{OL} \leq 5 \%$	24	0	3	0	0	0	0	0	0	0
$5 \% < \text{OL} \leq 6 \%$	4	0	0	0	0	0	0	0	0	0
$6 \% < \text{OL} \leq 7 \%$	2	0	0	0	0	0	0	0	0	0
$7 \% < \text{OL} \leq 8 \%$	1	0	0	0	0	0	0	0	0	0
Maximum overlap	7.48	2.69	4.45	2.16	1.01	1.22	0.22	1.09	0.11	0.07
Average overlap	1.01	0.7	0.39	0.58	0.09	0.55	0.02	0.64	0.02	0.01
Number overlaps	91061	1422	71011	971	66758	703	60517	622	112462	4200
Bulk porosity	0.3522		0.3717		0.3696		0.3703		0.3812	
Number of balls	30001		30003		30001		30002		43223	

The axial variation in the average cross-sectional porosity for the HTTU ($E = 11.7 \text{ GPa}$) and the AP-HTTF packed bed models are shown in Figure 3.3. The axial variation in porosity was determined using Equation (3.10) with an axial increment of $0.01d_p$.

It can be observed in Figure 3.3 that the results for the two models are in good agreement with each other in the bottom near-wall and bulk regions. It should be noted that Van Antwerpen *et al.* (2012) defined the first half sphere diameter next to the wall as the wall region and the region between half a sphere diameter and five sphere diameters from the wall as the near-wall region. Unless specifically mentioned otherwise, in this paper the near-wall region will be considered to include the wall region. The values of the minimum porosities associated with the first second, third and fourth layers in the near-wall region for the HTTU model are respectively 26.8 %, 8.3 %, 11.2 % and 7.6 % less than corresponding values for the AP-HTF model. The minimum porosities in the near-wall region occur at the centres of the layers of spheres constituting the near-wall region. The porosity for the HTTU model in the bulk region between $0.4 \text{ m} < z < 1.3 \text{ m}$ is on average 2.5 % less than the porosity for the AP-HTTF model. It could be postulated that the spheres in the near-wall region in the case of the AP-HTTF model might be closer packed due to the fact that height of the AP-HTTF packed bed is 2.5 m compared to the height of 1.58 m of the HTTU packed bed.

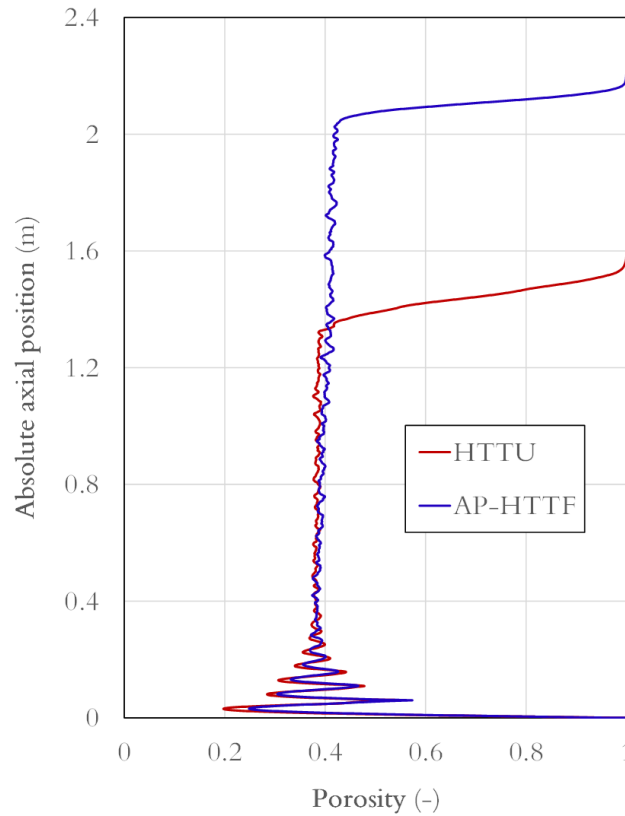


Figure 3.3: Axial variation in average cross-sectional porosity for the HTTU and AP-HTTF packed bed models.

The radial variation in the porosity for the HTTF-1 and HTTF-2 experiments (Du Toit, 2008), the HTTU (with $E = 11.7$ GPa) and the AP-HTTF packed bed models and the radial porosities predicted by the De Klerk correlations as per eqns. (3.15) and (3.16) are shown in Figure 3.4. The bulk porosity for the De Klerk in eq. (3.16) was taken as $\varepsilon_b = 0.3702$ from the HTTU with $E = 11.7$ GPa result as given in Table 3.1. Note that the radial positions were scaled using the annular width. The HTTF-1 and HTTF-2 experiments, AP-HTTF model, and the De Klerk (2003) predictions were based on the concept annular width of $14.167d_p$, whilst the HTTU model was based on the annular width of $14.065d_p$ taken from the design drawings. In the case of the HTTU ($E = 11.7$ GPa) and AP-HTTF models only the axial bulk region $0.4 \text{ m} < z < 1.2 \text{ m}$ was considered and the radial variation in porosity was determined using eq. (3.12) with a radial increment of $0.01d_p$. It can be observed in Figure 3.4 that the agreement between the HTTU, AP-HTTF and the De Klerk results for the outer near-wall region is better than for the corresponding results for the inner near-wall region. It could again be postulated that spheres in the near-wall regions in the case of the AP-HTTF model might be closer packed compared to the spheres in the near-wall regions in the HTTU model, resulting in larger amplitudes for the near-wall oscillations. Except for the first layers next to the inner and outer walls, the amplitudes of the oscillations in the case of the De Klerk correlations are larger than those associated with the HTTU and AP-HTTF models. Also, in the inner near-wall region the oscillations

associated with the De Klerk correlation gradually become out of phase with the corresponding oscillations for the HTTU and AP-HTTF models. Despite the scatter in the HTTF-1 and HTTF-2 experimental results, it can be cautiously observed that the agreement between the experimental results and the HTTU radial profile is better than the corresponding comparison between the experimental results and the AP-HTTF radial profile. In general, it can be stated that the agreement between the numerical and the experimental results is good. The De Klerk correlations eq. (3.15) and (3.16) should be used with the necessary caution to predict the radial variation in porosity of the HTTU annular packed bed.

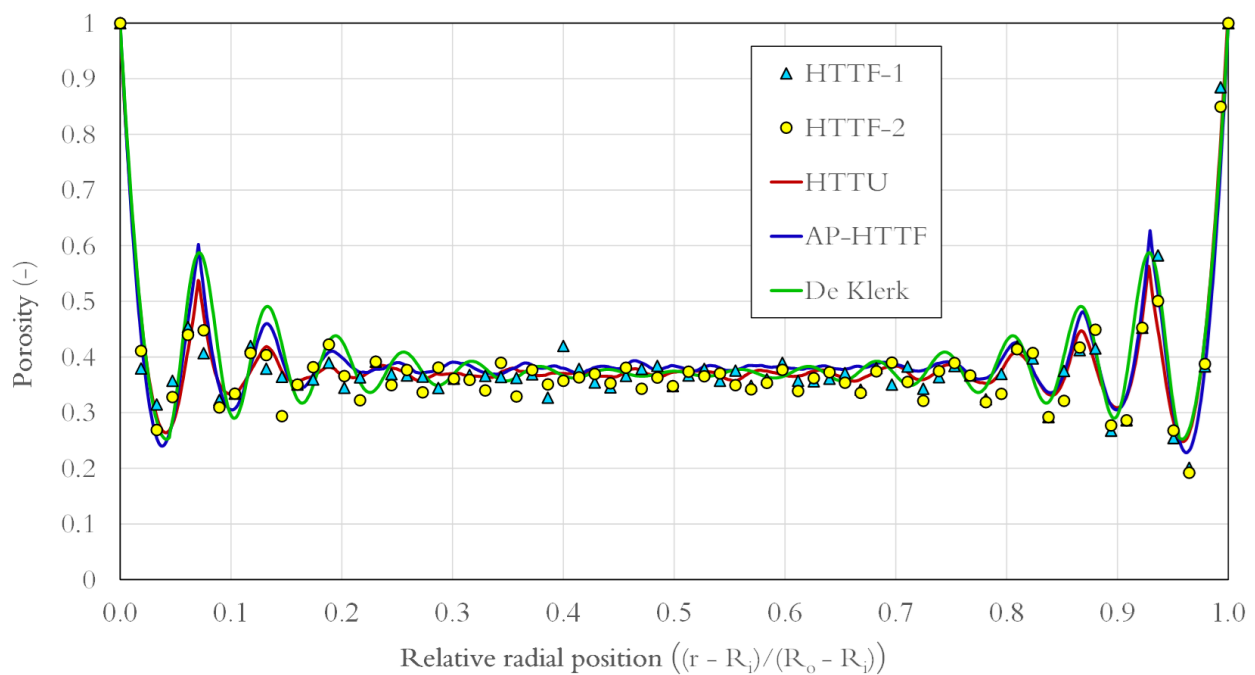


Figure 3.4: Radial variation in porosity for the HTTF-1 and HTTF-2 experiments, HTTU and AP-HTTF models and the De Klerk correlations.

It may therefore be concluded that the DEM (numerically) generated HTTU model can be considered as representative of the HTTU annular packed bed and therefore be analysed further to explore selected characteristics of the porous structure of the HTTU's annular packed bed. This model is also used directly as the geometry which is used for the isothermal flow and the forced convection CFD models described in Chapter 4.

3.3.2. Radial variation of the porosity of the axial layers in the bottom near-wall region

The next step in the analysis of the numerically generated HTTU annular packed bed model is to evaluate the radial and angular variation in porosity of selected sphere layers and sphere rings in the bottom near-wall region.

Figure 3.5 shows the positions of the centres of the spheres in the HTTU annular packed bed model plotted on the x - y plane in Figure 3.5(a) and plotted on the r - z plane in Figure 3.5(b). The radial position r_i of sphere i is given by $r_i = \sqrt{x_i^2 + y_i^2}$. Figure 3.5(a) should be viewed in conjunction with Figure 3.4, whilst Figure 3.5(b) should be viewed in conjunction with Figure 3.3 and Figure 3.4. In Figure 3.5(a) the radial rings in the inner and outer near-wall regions can be observed. The axial sphere layers in the bottom near-wall region and the radial sphere layers or rings, in the inner and outer near-wall regions, can be seen in Figure 3.5(b). Figure 3.5(b) also gives an indication of the interference between the axial layers and radial rings. These results show the same characteristics as corresponding results for a cylindrical pack bed presented by Reimann *et al.* (2017).

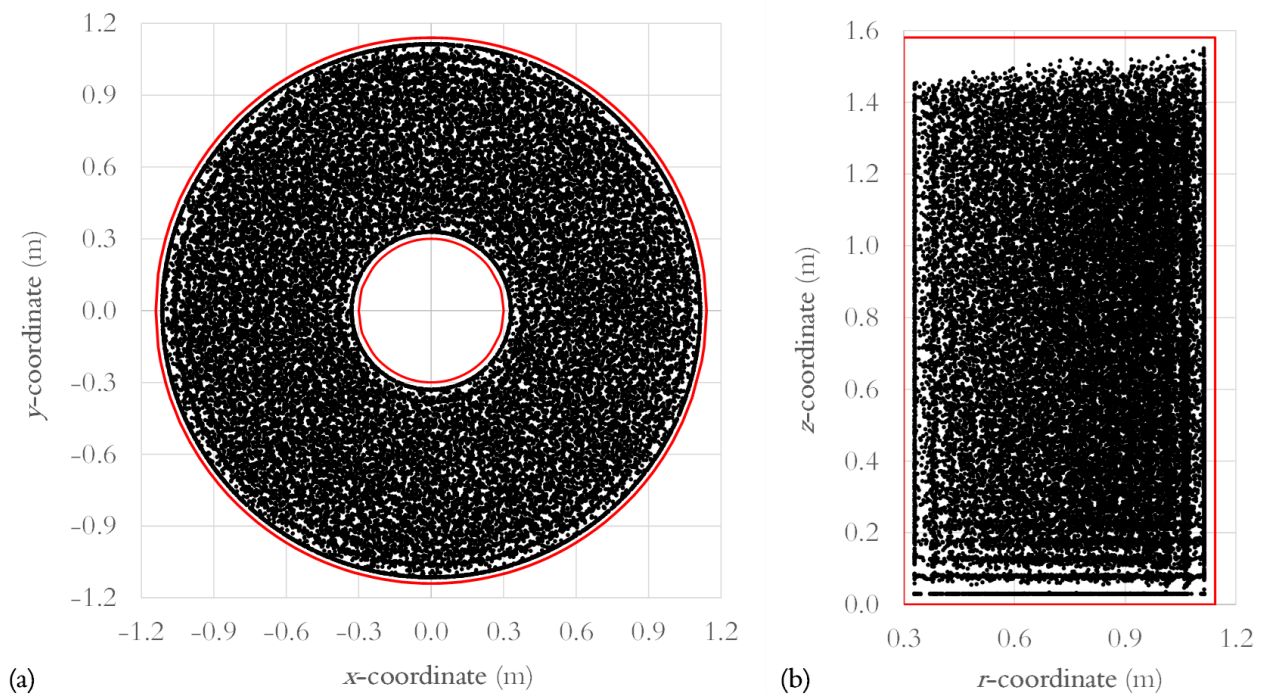


Figure 3.5: Sphere centre coordinates in the HTTU annular packed bed model on the x - y (a) and r - z plane (b).

The bottom, centre and top of each of the seven axial layers that can be identified in Figure 3.3 are summarised in Table 3.2. The interface (top/bottom) between two successive layers occurs where $(\partial\epsilon/\partial z)_i > 0$ and $(\partial\epsilon/\partial z)_{i+1} < 0$, and the centre of a layer occurs where $(\partial\epsilon/\partial z)_i < 0$ and $(\partial\epsilon/\partial z)_{i+1} > 0$.

The height or thickness of each layer is given in the last column. Note that all the values are normalized with respect to the sphere diameter. It can be observed in Table 3.2 that the first layer is approximately 20 % thicker than the second, third and fifth layers, 23 % thicker than the fourth layer, and 24 % thicker than the sixth layer. The larger thickness of the seventh layer, compared to the previous five layers, can be attributed to the fact that it can be considered as the transition layer to the bulk region. The values of the thickness are an indication of the interpenetration of the layers as result, amongst others, of the spheres in a layer fitting into the gaps or indentations between the spheres of the layer below it.

Table 3.2: Axial positions of axial layers in the bottom near-wall region.

Layer	Axial distance from bottom (z/d_p)			Height ($\Delta z/d_p$)
	Bottom	Centre	Top	
First	0.0000	0.5199	1.0099	1.0099
Second	1.0099	1.3399	1.8198	0.8099
Third	1.8198	2.1498	2.6197	0.7999
Fourth	2.6197	2.9697	3.3896	0.7699
Fifth	3.3896	3.7496	4.1896	0.7999
Sixth	4.1896	4.5595	4.9495	0.7599
Seventh	4.9495	5.3094	5.8294	0.8799

The positions of the inner edge, centre, and outer edge of the first three rings in the inner and outer near-wall regions are summarised in Table 3. The interface (outer/inner edge) between two successive rings occurs where $(\partial\epsilon/\partial r)_i > 0$ and $(\partial\epsilon/\partial r)_{i+1} < 0$, and the centre of a ring occurs where $(\partial\epsilon/\partial r)_i < 0$ and $(\partial\epsilon/\partial r)_{i+1} > 0$. The widths of the rings are also given in Table 3.3. Note again that all the values are normalized with respect to the sphere diameter.

Table 3.3: Radial positions of first three radial sphere rings of the inner and outer near-wall regions.

Ring	Inner near-wall region				Outer near-wall region			
	Distance from wall $((r-r_i)/d_p)$			Width $(\Delta r/d_p)$	Distance from wall $((r_o-r)/d_p)$			Width $(\Delta r/d_p)$
	Inner	Centre	Outer		Inner	Centre	Outer	
First	0.0000	0.5802	0.9803	0.9803	1.0103	0.5702	0.0000	1.0103
Second	0.9803	1.3905	1.8506	0.8703	1.8706	1.4105	1.0103	0.8603
Third	1.8506	2.2107	2.6409	0.7903	2.6909	2.2407	1.8706	0.8203

It can be observed in Table 3.3 that in the case of inner near-wall region the first ring is 11 % wider than the second ring and 19 % wider than the third ring. In the case of the outer near-wall region the first ring is 15 % wider than the second ring and 19 % wider than the third ring. The values of the widths are also an indication of the interpenetration of the rings as result, amongst others, of the spheres in a ring fitting into the gaps or indentations between the spheres of the ring nearer to the wall.

Figure 3.6 depicts the angular variation in porosity for $0 \leq \theta \leq 45^\circ$ for the (a) first, (b) second and (c) third layers of the first ring; for the (d) first, (e) second and (f) third layers of the second ring, of the outer near-wall region. The angular variations in porosity were obtained employing (3.11) and an angular increment of $\Delta\theta = 0.1^\circ$ was used. For the first ring it is the equivalent of approximately 30 increments per sphere. Figure 3.6 (a) is associated with the ring of spheres in the corner between the outer wall and the bottom of the annulus. It can be seen that the spheres are regularly packed, except for the sphere at 22.5° which apparently could not fit fully between the adjacent spheres. In Figure 3.6 (b) it can be seen that the spheres have rotated a half sphere diameter with respect to the spheres in the first layer. The spheres in the third layer are again rotated a half sphere diameter with respect to the spheres in the second layer as can be seen in Figure 3.6 (c). The packing of the spheres in the second and third layers is less regular than for the first layer. The same pattern is observed in Figure 3.6 (d), (e) and (f) for the second ring. It can also be observed that the spheres in the second ring are rotated a half sphere diameter with respect to the spheres in the first ring. The rotation of the layers and second rings occur for the spheres in the layer or ring to fit into the gaps or indentations between the spheres in the adjacent layer or ring. The packing of the spheres become more irregular as the distance between the layers and rings considered and the bottom and wall increases.

The average porosity for each of the layers for was calculated using Simpson's Rule (Kreyszig, 2006), as well as the standard deviation using eq. (3.13) and the skewness using eq. (3.14). The results are summarised in Table 3.4.

Table 3.4: Average porosity, standard deviation, and skewness of first three axial layers of the first and second radial sphere rings of the outer near-wall region.

Layer	First ring			Second ring		
	$\bar{\epsilon}$	σ	μ	$\bar{\epsilon}$	σ	μ
First	0.2158	0.2287	1.4417	0.2621	0.2501	1.1048
Second	0.2226	0.2836	1.2795	0.3191	0.3085	0.8038
Third	0.2161	0.2677	1.2425	0.2505	0.2599	1.0750

It can be seen in Table 3.4 that the average porosities of the second ring are larger than those for the first ring indicating the spheres in the second ring are less closely packed than the spheres in the first ring against the wall. It can also be seen in Table 3.4 that the magnitudes of the average porosities and the corresponding standard deviations are almost the same indicating a large variation in the porosity. This is confirmed by the variation in porosity observed in Figure 3.6. The values of the skewness in Table 3.4 show that the variations in the porosities are highly positively skewed indicating that the average porosity is larger than the median porosity.

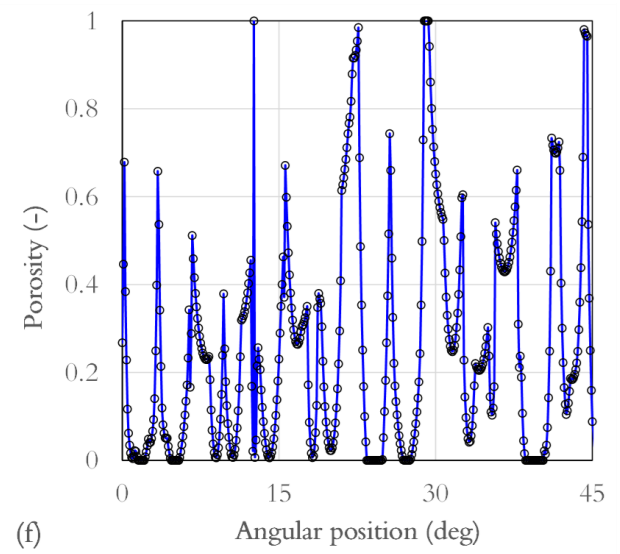
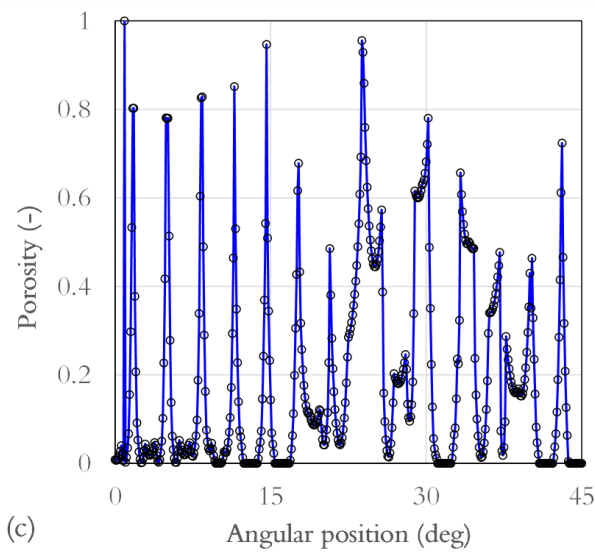
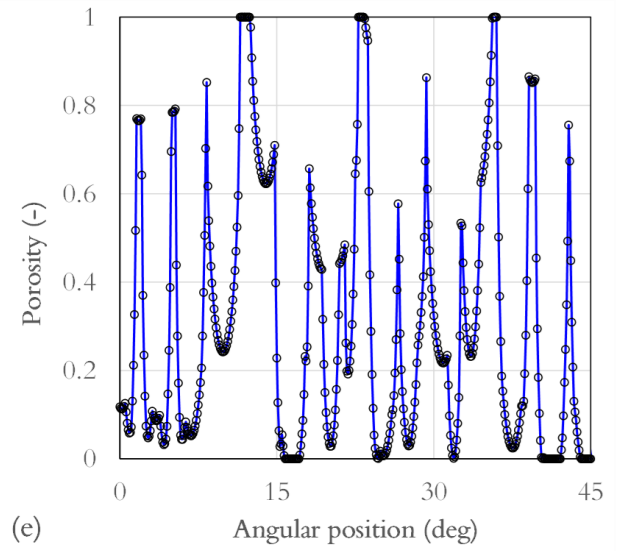
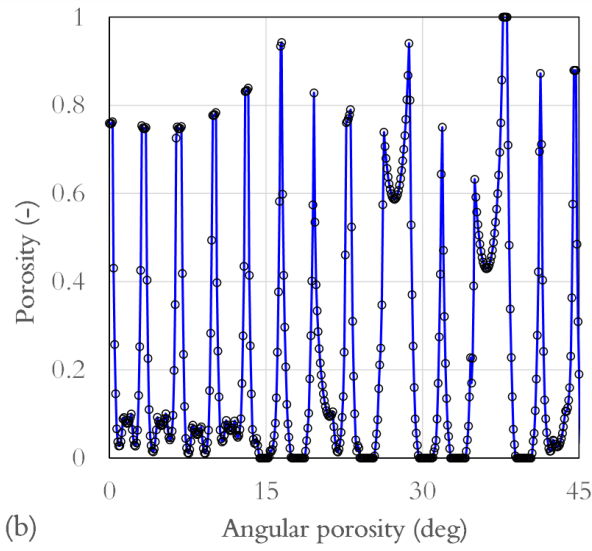
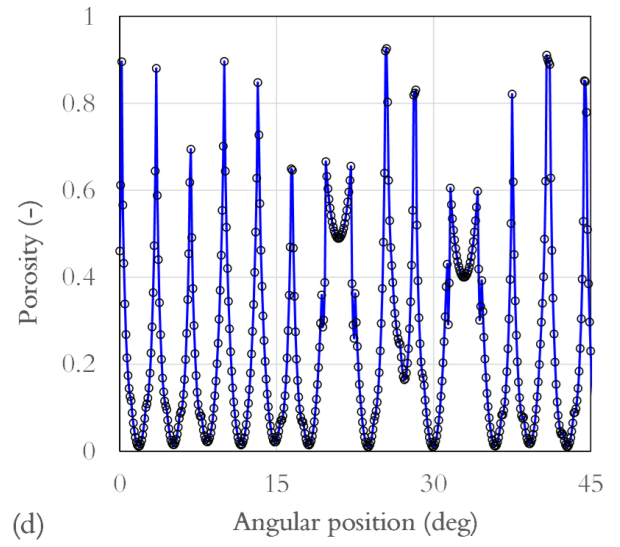
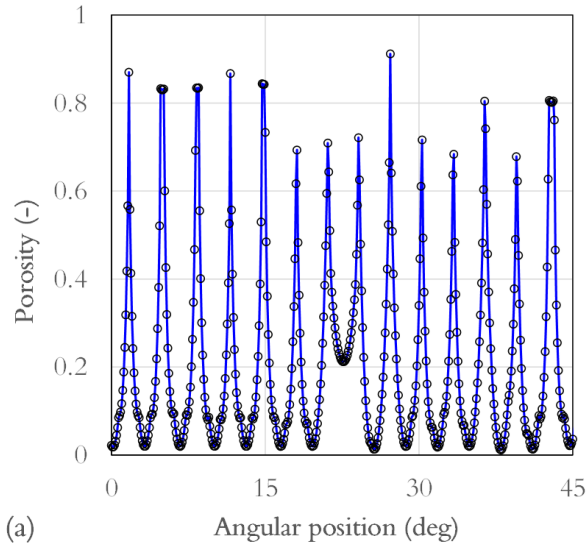


Figure 3.6: Angular variation in porosity for $0 \leq \theta \leq 45^\circ$ for the first, second and third layers of the first ring (a), (b), (c) and second ring (d), (e), (f), respectively, of the outer near-wall region.

The next to step to gain further insight into the characteristics of the porosity in the bottom near-wall region, was to study a single layer. For this purpose, the third layer was selected. Eqns. (3.12), (3.13) and (3.14) were employed to obtain the radial variation porosity, standard deviation and skewness, respectively.

Figure 3.7 shows (a) the radial variation in porosity, (b) the standard deviation and (c) the skewness. Three cases were considered: in the first ("layer" in Figure 3.7) the thickness of the layer was taken from the bottom of layer three to the top of layer three, as given in Table 3.2. For the second ("layer plus half" in Figure 3.7) the thickness of the layer was taken from the centre of layer two to the centre of layer four, as given in Table 3.2. In the third case ("layer plus one" in Figure 3.7) the thickness of the layer was taken from the bottom of layer two to the top of layer four. It can be observed in Figure 3.7 (b) that the standard deviations for the "layer plus half" and "layer plus one" are about 60 % of the standard deviation for the "layer" in the region excluding the wall regions. The skewness for the "layer" is also noticeably larger than the skewnesses for the "layer plus half" and "layer plus one" as can be seen in Figure 3.7 (c).

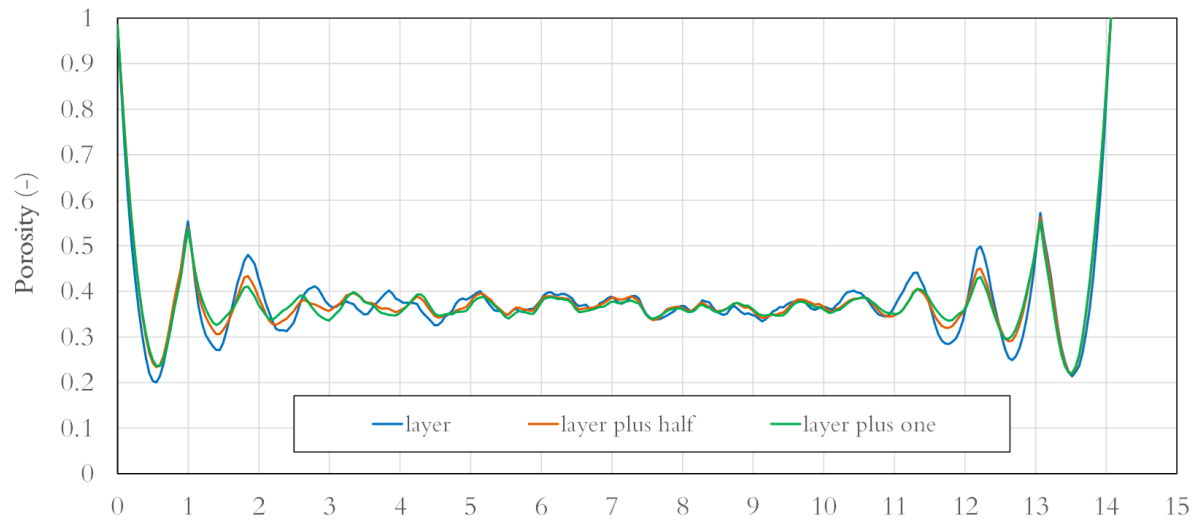
The differences between the porosities for the three cases are less marked. The same characteristics are exhibited by layers two and four to six. The average porosities and average standard deviations for layers one to four considering a layer only and a layer plus half are summarised in Table 3.5. The marked change in the average standard deviation between a layer and layer plus half analysis can be seen in Table 3.5.

Table 3.5: Average porosity and standard deviation for first four layers in bottom near-wall region.

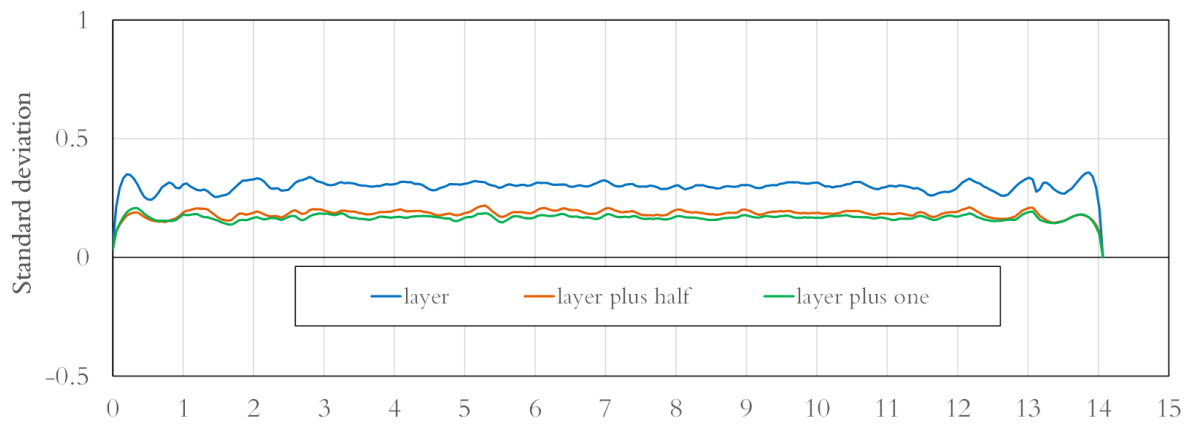
Layer	Layer only		Layer $\pm$ half layer		% change	
	$\bar{\epsilon}$	$\bar{\sigma}$	$\bar{\epsilon}$	$\bar{\sigma}$	$\bar{\epsilon}$	$\bar{\sigma}$
First	0.4136	0.2830	0.4032	0.2175	-2.5	-23.1
Second	0.3762	0.3108	0.3696	0.1835	-1.8	-41.0
Third	0.3753	0.2989	0.3781	0.1834	0.7	-38.6
Fourth	0.3795	0.2983	0.3793	0.1863	-0.1	-37.6

It could be argued that considering a layer alone does not sufficiently account for the effects of the inter-penetration of the layers. It is therefore suggested that when a layered approach is followed for the description of the porosity in the bottom near-wall region, that it be based on a "layer plus half" analysis. This could be considered as akin to a running average.

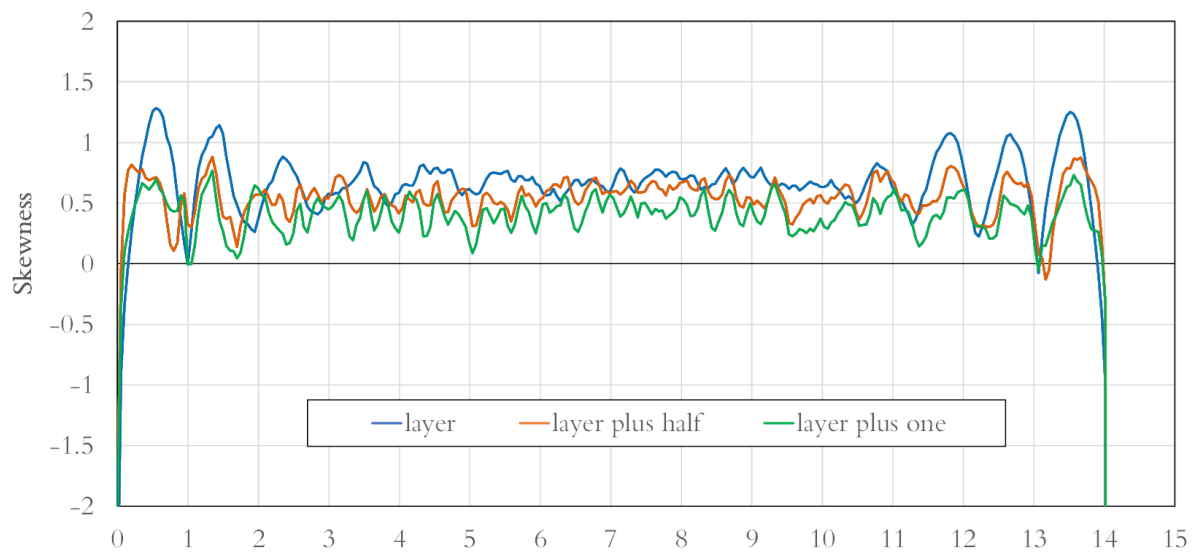
The radial variation in the porosity for layers one to four in the bottom near-wall region based on a "layer plus half" analysis is shown in Figure 3.8.



(a) Distance from inner wall $((r-R_i)/d_p)$



(b) Distance from inner wall $((r-R_i)/d_p)$



(c) Distance from inner wall $((r-R_i)/d_p)$

Figure 3.7: Radial variation in the (a) porosity, (b) standard deviation and (c) skewness for the third layer in the bottom near-wall region.

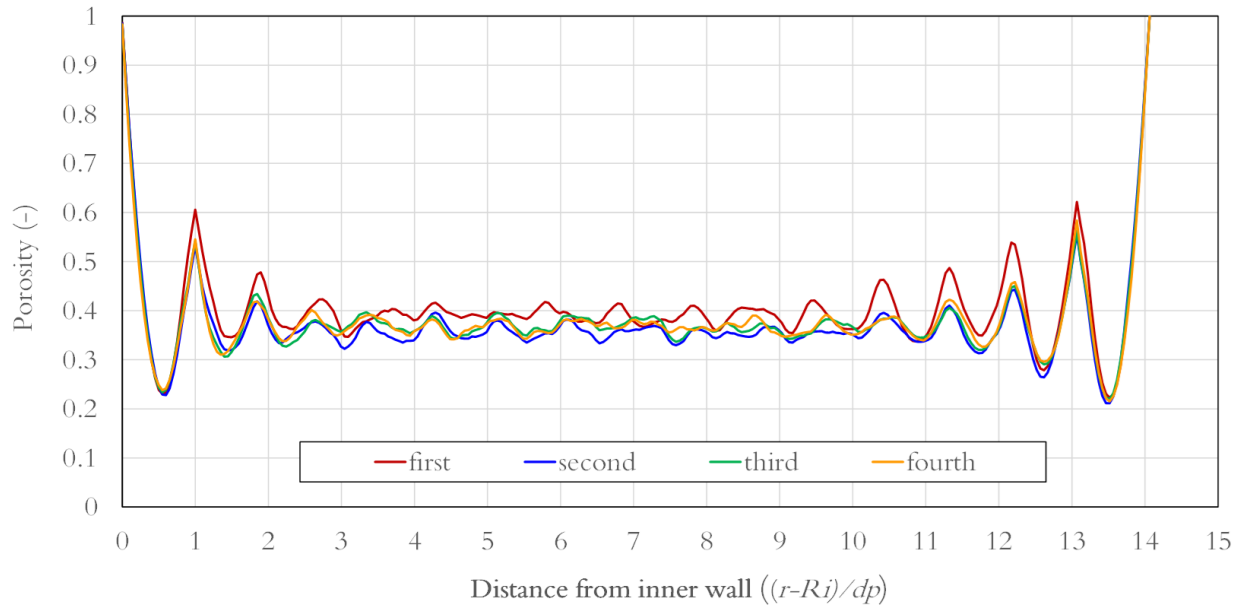


Figure 3.8: Radial porosity variation for layers one to four in the bottom near-wall region.

The radial variations in porosity for layers two to four are in good agreement, whilst the effects of the wall regions associated with the inner and outer walls, and the bottom wall on the radial variation of the first layer can be seen in Figure 3.8. From the results it could be deduced that it is only necessary in the case of the first layer in the bottom near-wall region to use a unique description for the radial variation in the porosity.

3.3.3. Porosity distribution in axi-symmetric r - z plane

The analysis of the radial variation of the porosity in the bottom near-wall region discussed in Section 3.3.2 does not reflect the interference between the axial layers in the bottom near-wall region and the rings in the inner and outer near-wall regions that can be observed in Figure 3.5(b). To investigate the radial and axial variation in porosity in more detail, a grid of (r_i, z_i) points with a spacing of $0.1d_p$ in both the r - and z -directions was defined. The tangentially averaged porosity for each point was determined using eq. (3.19) and the resulting porosity distribution can be considered as the variation in porosity on an axi-symmetric r - z plane and is shown in Figure 3.9.

The rings in the inner and outer near-wall regions and the layers in the bottom near-wall region, as well as the interference between the rings and the layers can be observed in Figure 3.9. In the visualization of Figure 3.9 it should be remembered that the centres of the layers and rings correspond to regions of minimum porosity, whilst the interfaces between layers and between rings correspond to regions of maximum porosity.

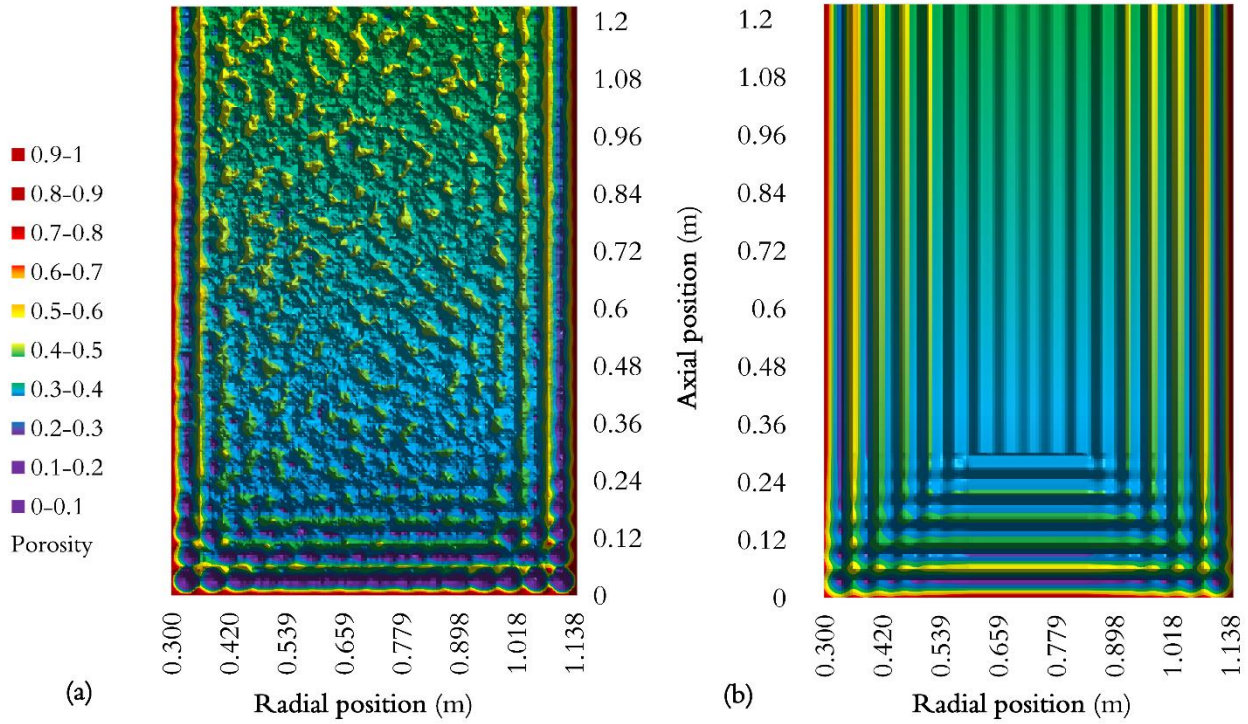


Figure 3.9: Variation of the tangentially averaged porosities on an axis-symmetric r - z plane (a) and variation of the predicted porosities on an axis-symmetric r - z plane (b).

For example, the line of features approximately a half sphere diameter from the bottom wall are depressions of minimum porosity where the rings associated with the inner and outer walls interfere with the first layer next to the bottom wall. Thus, the depression at $r \approx 0.33$ m and $z \approx 0.03$ m is the interference between the first ring from the inner wall and the first layer from the bottom wall. The approach used to obtain Figure 3.9 provides more detail on the variation of the porosity than the approach employed by Suikkanen *et al.* (2014) who could only obtain a piecewise Voronoi cell constant distribution for the porosity. The advantage, however, of the approach used by Suikkanen *et al.* (2014) is that it provides a three-dimensional variation of the porosity.

There are two possibilities how the porosity results depicted in Figure 3.9 can be implemented in a porous medium CFD model. In both cases it is assumed that individual porosity values can be assigned to the computational cells or grid points. In the case where a code has the capability to map scalar values from one grid onto another grid, the values associated with the porosity grid, for example the grid used in Figure 3.9, can be imported into the CFD model, and then mapped as required. Alternatively, the coordinates of the cell centres or grid points associated with the CFD model can be exported and imported into the porosity. After the porosities have been calculated, the porosity results associated with the cell centres or grid points are then imported into the CFD model.

When the coordinates of the spheres constituting the packed bed are not available, the approach discussed by Reyneke & Du Toit (2010) can be employed to generate the porosities associated with grid points defined on the axi-symmetric r - z plane. Based on the finding of Van Antwerpen *et al.* (2010) that the correlations of De Klerk (2003) are the most suitable correlations to predict the radial variation of the porosity for the HTTU annular packed bed, eqns. (3.15) and (3.16) were used to predict the values of the porosities. Furthermore, Goodling *et al.* (1983) found that the effect of a wall on the variation in porosity can be detected up to five sphere diameters from the wall.

When $y^* < 5$ and $z^* < 5$, thus in the inner or outer near-wall region and the bottom near-wall region, Reyneke & Du Toit (2010) proposed that the porosity can be obtained as the weighted average of the radial and axial porosities and given as:

$$\varepsilon(r, z) = \frac{(5 - y^*)\varepsilon(y^*) + (5 - z^*)\varepsilon(z^*)}{(5 - y^*) + (5 - z^*)} \quad (3.20)$$

with

$$y^* = \min \left[\frac{R_o - r}{d_p}, \frac{r - R_i}{d_p} \right] \quad (3.21)$$

When $y^* \geq 5$ and $z^* < 5$, thus only in the bottom near-wall region, then

$$\varepsilon(r, z) = \varepsilon(z^*) \quad (3.22)$$

When $z^* \geq 5$ and $z < z_b$ where z_b is the axial position of the top of the bulk region, then the porosity is only affected by the inner and outer walls and is given as:

$$\varepsilon(r, z) = \varepsilon(y^*) \quad (3.23)$$

Finally, when $z \geq z_b$, thus in the top region of the packed bed, then

$$\varepsilon(r, z) = 1.0 - \left[1.0 - \varepsilon(y^*) \right] \cdot \frac{H - z}{H - z_b} \quad (3.24)$$

where H is the height of the packed bed.

The variation of the predicted porosities on an axi-symmetric r - z plane based on eqns. (3.15), (3.16) and (3.20) to (3.24) is shown in Figure 3.9(b) and the interference between the rings in the inner and outer near-wall regions and the bottom near-wall region can be observed. When the porosity distribution in Figure 3.9(b) is compared with the porosity distribution in Figure 3.9(a), it can be seen that it exhibits the same characteristics. However, the effects of the random, or irregular packing of the spheres away from the bottom and the inner and outer walls are not represented in the porosity distribution in Figure 3.9(b).

Nevertheless, it can be concluded that in the absence of detailed information on the positions of the spheres in the annular packed bed, the proposed approach provides a representative description of the variation of the porosity on an axi-symmetric r - z plane of the annular packed bed that can be implemented in a porous medium CFD model.

3.3.4. Average regional porosities and standard deviations

Typically, the computational domain in a CFD simulation is divided into regions and the relevant properties, including the porosity in the case of a porous medium model, are then assigned to each region in the form of constant values or correlations. When the computational mesh is generated a cell or an element then obtains the required properties from the values assigned to the region in which it resides. Thus, to implement the variation in porosity as described in Section 3.3.3 will require that each cell or element be defined as a region. This can complicate the setting-up of the computational model considerably.

Therefore, following the examples of Reimann *et al.* (2017), Du Toit (2019a) and Bester & Du Toit (2022), the HTTU annular packed bed model was divided into four axial regions and five radial regions to account for the variation in porosity in such a situation. In axial direction the annular packed bed was divided into the bottom wall region (BW), $0.0 \text{ m} < z < 0.0312 \text{ m}$; bottom near-wall region (BNW), $0.0312 \text{ m} < z < 0.3768 \text{ m}$; bottom bulk region (BB), $0.3768 \text{ m} < z < 1.20 \text{ m}$; and the bottom top region (BT), $1.20 \text{ m} < z < 1.5802 \text{ m}$. In radial direction the annular was divided into the inner wall region (IW), $0.30 \text{ m} < r < 0.3342 \text{ m}$; inner near-wall region (INW), $0.3342 \text{ m} < r < 0.5887 \text{ m}$; bulk region (B), $0.5887 \text{ m} < r < 0.8426 \text{ m}$; outer near-wall region (ONW), $0.8426 \text{ m} < r < 1.1097 \text{ m}$; and the outer wall region (OW), $1.1097 \text{ m} < r < 1.1439 \text{ m}$.

Eqns. (3.17) and (3.18) were then used to calculate the average porosity and the standard deviation for each of the 20 regions. For each region the radial limits $r_l \leq r \leq r_2$ and the axial limits $z_l \leq z \leq z_h$ corresponded to the values given in the previous paragraph, whilst the angular limits were defined as $0 \leq \theta < 2\pi$. The values of the average porosity and the standard deviation obtained for each region are summarised in Table 3.6. The effect of the bottom, inner and outer walls, and the top can be seen in the larger values for the average porosities and the standard deviation. The values of the average porosity and standard deviation for the near-wall and bulk regions are in good agreement. The results for the average porosity for the radial regions in the BW, BWN and BB axial regions reflect the results shown in Figure 3.4 and Figure 3.8. In CFD codes that have the capability to account for the uncertainties associated with properties, the standard deviation can be employed to assign uncertainties to the values of the porosity.

Table 3.6: Average regional porosity and standard deviation distribution for radial and axial regions.

		IW	INW	B	ONW	OW
BT	$\bar{\epsilon}$	0.6859	0.5978	0.5911	0.6165	0.7183
	σ	0.1593	0.0994	0.1112	0.1326	0.1873
BB	$\bar{\epsilon}$	0.4948	0.3725	0.3704	0.3735	0.5141
	σ	0.2270	0.0777	0.0702	0.0833	0.2445
BNW	$\bar{\epsilon}$	0.4833	0.3689	0.3637	0.3694	0.4929
	σ	0.2472	0.1134	0.1068	0.1170	0.2578
BW	$\bar{\epsilon}$	0.4935	0.4606	0.4599	0.4722	0.4863
	σ	0.3577	0.3310	0.3306	0.3345	0.3557

Should it be required, the HTTU annular packed bed can also be divided into regions in the angular direction, as done by Bester & Du Toit (2022), to provide a piece-wise regional constant three-dimensional variation of the porosity and the associated standard deviation.

3.4. Chapter Conclusions

In the nuclear industry, in several reactor designs the core is a packed bed of equal sized spheres (IAEA, 2013). The flow, pressure drop, and heat transfer characteristics of a packed bed are dependent on the packing structure (Kugeler & Schulten, 1989); (KTA, 1983); (Rodríguez, *et al.*, 2021). The most important characteristic of the porous structure is the porosity (Suikkanen, *et al.*, 2014); (Von Seckendorff, *et al.*, 2021). A proper understanding of the porosity and how it affects the phenomena that determine the performance of the packed bed reactor is therefore essential (Novak, *et al.*, 2019).

In this chapter a comprehensive characterization of the variation in the porosity of HTTU annular packed bed was presented as an extension of the previous work of Du Toit (2008), Reyneke & Du Toit (2010) and Du Toit (2019a) and published in article form in (Potgieter & Du Toit, 2023). A numerical model of the HTTU annular packed bed consisting of equal sized spheres was generated using the DEM code *ESSS Rocky*, version 4.3 (ESSS, 2022). The semi-analytical and numerical methods developed by Du Toit (2019b) and Bester & Du Toit (2022) were employed to determine the porosity of the HTTU annular packed bed consisting of equal sized spheres. The methods require that the coordinates of the centres of spheres and the diameters be known. The semi-analytical methods were extended to be able to also calculate the skewness of the angular variation in porosity a given radial position. Furthermore, the x - y grid porosity method developed by Bester & Du Toit (2022) was adapted to obtain the axi-symmetric (tangentially averaged) porosity on an r - z plane by employing the tangentially averaged horizontal line-based method developed by Mueller (2012) and Du Toit (2019b).

The methodology developed by Bester & Du Toit (2022) to calculate the average porosity of a wedge was also extended to include the calculation of the standard deviation of the porosity for the wedge.

As a first step the quality and the representativity of the numerically generated HTTU annular packed bed was evaluated. This was firstly done by considering the overlaps between the spheres and between spheres and the walls. The results were compared with the corresponding results of the AP-HTTF annular packed bed, as well as HTTU packed beds for which smaller Young's moduli were employed. It was found that there is a very good correspondence between the results for the HTTU and AP-HTTF annular packed bed. Secondly the axial variations in porosity for the HTTU and AP-HTTF were compared and found to be in good agreement in the bottom near-wall and bulk regions. Lastly the radial variation in porosity for the HTTU annular packed was compared with radial variations in porosity for the HTTF-1 and HTTF-2 experiments and the AP-HTTF numerical packed bed (Du Toit, 2008). In general, the agreement is good. It was concluded that the HTTU numerical packed bed model can be considered as representative and can thus be used for further analysis.

As a second step the radial variation in porosity of the axial layers constituting the bottom near-wall region was evaluated. The axial layers, as well as the radial rings of spheres were identified from plots showing the positions of the centres of the spheres, as well as the axial and radial variations in porosity. Plots of the angular variation in porosity for the first three axial layers and first two rings next to the outer wall show how the layers and rings are staggered with respect to each other. The analysis of the radial variation in porosity also included the standard deviation and the skewness of the angular porosity at each radial position. An analysis of the radial porosity of the layers revealed only first layer next to the bottom is markedly affected by the bottom wall.

The plot of the centres of the spheres in terms of their radial and axial positions revealed the presence of interference between the radial variations in the porosity from the inner and outer walls and the bottom wall. The study of the radial variation in porosity in the bottom near-wall region, however, did not shed any light on this. To consider this in more detail a grid of r - z points on an axi-symmetric plane was defined and the tangentially averaged porosity for each point was calculated. The resultant plot of the porosity values showed the effect of the interference between the various wall layers and rings on the variation in the porosity. Where possible these grid values of the porosity can be mapped onto a porous medium CFD mesh to account for the variation in porosity in the thermal-hydraulic simulation. It was also shown that a similar r - z plot of the porosities can be obtained from the weighted average of the radial and axial porosities calculated using an oscillatory porosity correlation such as that proposed by De Klerk (2003).

Following the methodology of Bester & Du Toit (2022) the computational domain was divided axially and radially into regions and that average porosity and the standard deviation of the porosity for each region were calculated. These regional values for the porosity and the standard deviation of the porosity can be implemented in a porous medium CFD model by defining these regions in the set-up of the mesh and assigning the relevant porosity and standard deviation values to the mesh regions.

Lastly, the variation in solid fraction could also be applied in other more ambitious studies, such as a coupled model to evaluate the influence of the packing structure on annular pebble bed core neutronics and the occurrence of hot spots due to local differences in reactivity.

End of Chapter



4. METHODOLOGY AND MODEL SET-UP

This Chapter proceeds to discuss the approach to modelling the annular packed bed of the HTTU experiment, consisting of several thousand uniform spheres, in a pragmatic way. It outlines the parameters, boundary conditions and assumptions made in the set-up of both a porous media model of a full bed, relying on correlations, as well as a discrete CFD model of a section of bed, which solves the fluid and solid domains explicitly.

4.1. Choice of Numerical Model

As discussed in Chapter 2, there are several methods both past and present to model the physical phenomena in pebble beds. For a homogenised and bed-averaged model, a purely analytical approach may be applied for low effort calculations. For numerical modelling, there are two approaches considered: semi-analytical where some correlations are used, and fully resolved numerical. In this section the merit of applying each approach to a model of the HTTU is discussed.

4.1.1. Analytical Approach

Analytical formulae such as detailed in Section 2.3 are generalisations derived from the evaluation of experimental measurements or observations and therefore provide answers with a relatively high reliability and accuracy when applied to problems with similar bounds in terms of key defining parameters to that of the experiments they are based on. Where pebble beds are concerned, these would include but are not limited to the bed porosity, gas flowrates (therefore Reynolds numbers), and temperatures.

Where the physical case deviates significantly from the experimental, analytical methods tend to lead to large uncertainties and inaccuracy. As was observed in the porosity evaluation in Section 3.3, that the assumption of an average porosity is not valid in the wall and near-wall regions, roughly 3 sphere diameters from a wall. With the HTTU being of an annular geometry with 60 mm spheres, this translates to 180 mm from the inner and outer reflectors. In total, for 360 mm of the overall 850 mm of the radius or 42 %, where the assumption of an average porosity would not hold true. This of course depends on the distance used to calculate an integral average and overall, the oscillatory value of porosity averages around the expected value, but on a scale that pertains to the coolant flow and heat transfer phenomena, the local larger variation in porosity does play a significant role: approaching $\varepsilon = 1$ at the wall.

One approach could be to discretise the analytical bed in radial sections with a porosity value closer to that of the physical bed, but this may lead to applying the formulae with values for which they have not been validated. In the case of pressure drop as defined in KTA 3102.2 for example, the valid porosity values only range from 0.36 to 0.42 (KTA, 1983). Similarly, this would apply to the heat transfer when it is lumped in a convective coefficient as in KTA 3102.3 (1981) as well as correlations for the radiative heat transfer such as the MSUC (Van Antwerpen, 2009).

4.1.2. Numerical Approach with Discrete Geometry

With the exponential improvements in computational power as well as computer codes that can exploit the latest hardware, the application in terms of scale and depth in physics of CFD methods have grown exponentially. This is evident to the topic of this study as well as shown in Section 2.4.3.

Applying a finite volume method to the discrete flow domain of a pebble bed core allows explicit modelling of the turbulent gas flow and thereby account for convective heat transfer. Including other physics models such as surface-to-surface radiation and adding a solid domain with conduction allows an integral approach to the overall thermal-hydraulic problem.

This approach is the primary focus of this study and where most of the effort was spent to verify and validate its applicability to the set of experimental results. Another semi-explicit approach is also possible and was investigated, as described in the next sub-section.

4.1.3. Numerical Approach with Representative (Porous Medium) Geometry

Whilst the computational expense of CFD methods varies greatly between DNS, LES and RANS turbulence modelling (or fully resolving in the case of DNS) generally it is significant compared to the negligible solution times of analytical calculations. The total computational effort required is arguably not only because of the solving of the associated mathematical physics models, but the number of control volumes necessary to adequately describe the geometry of the problem in a way that allows solving or resolving the scale of physics within the domain. The comparative effort for 'simpler' physics over an equal number of volumes is much less, however the nuance is that more 'complex' physics requires a finer discretisation of the same geometry in order to adequately capture the scale of the underlying physics.

It therefore stands to reason that the required resolution of a computational method that uses correlations for the most significant physics need only be as fine as the distinguishing parameter for the correlation used before the gain in accuracy with finer resolutions results in diminishing returns. In the porous medium approach to a pebble bed geometry, this is mainly the porosity.

A second potential approach to the modelling of the HTTU packed bed presented in this study is to apply the validated correlations of the KTA to a porous medium domain in CFD with a rough discretisation of the porous zone into axial and radial sections of different porosities. For the sake of brevity, the approach of a representative porous domain with correlations will simply be referred to as the porous approach.

4.2. Description of the HTTU Experiment

4.2.1. Background

The PBMR company commissioned the construction of the High Temperature Test Facility to investigate the thermal-hydraulic phenomena of importance to a pebble bed reactor. The engineering, construction and operation of the facility was contracted to M-Tech Industrial (Pty) Ltd. and hosted on the Potchefstroom Campus of the North-West University as was done with the earlier Pebble Bed Micro Model (PBMM) (Greyvenstein, *et al.*, 2003). Several experiments were located in the facility with two of particular note being the High Pressure Test Unit (HPTU) and the High Temperature Test Unit (HTTU) (Rousseau & Van Staden, 2008).

4.2.2. Purpose

The PBMR-400 design utilised a direct helium Brayton cycle for energy conversion, as opposed to an indirect steam Rankine cycle. In order to operate at high efficiencies and because of the direct cycle the design aimed for a core outlet temperature of 900 °C, higher than was achieved with past pebble bed designs built for steam generation. As part of its development, the qualification program therefore had to cover sufficient experimental investigation at the high temperatures not covered in literature or past experience.

Primarily, therefore, the aim of the HTTU experiment was to investigate the thermal-hydraulic phenomena at the same temperatures expected in the first prototype. Because of the neutron flux and therefore thermal power distribution with a non-linear shape in respect to radial distance in a nuclear power reactor, an average outlet temperature of 900 °C would correspond to much higher peak temperatures. The objective with the HTTU was therefore to achieve a peak temperature of 1000 °C or higher (M-Tech Industrial, 2009d) but not to operate at the same high pressure of 9 MPa as the final design. In respect to the thermo-physical phenomena such as convection, conduction and radiation the HTTU experiments are considered integral effects tests.

4.2.3. Tests Campaign

The experimental campaign of the HTTU facility covered various tests at different flow, pressure and temperature conditions. In Table 4.1 and Table 4.2 below the different tests performed are summarised in matrix form. It should be noted that the forced flow tests are of interest to this study and all of these tests were performed using gaseous Nitrogen as coolant. No forced flow tests were done in the HTTU with gaseous Helium as coolant.

Table 4.1: Matrix of the forced flow tests completed during the HTTU experimental campaign.

Conditions	Power	Mass Flow (kg/s)				
Isothermal	-	0.5	1	2	3	4
Forced Convection	60 kW	0.5	1	2	3	4
	120 kW	0.5	1	2	3	4
	140 kW	0.5	1	2	3	4
	162 kW	0.5	1	2	3	4

The reasoning behind the selection of test cases and flow and heating parameters are not directly mentioned in the literature that was made available. It is however understood as mentioned below that the goal was to reach certain temperatures under different conditions.

Table 4.2: Matrix of the atmospheric and near-vacuum tests completed during the HTTU experimental campaign.

Conditions	Atmosphere	Power	Peak Temperature
Natural convection	Helium	20 kW	500 °C
		60 kW	1000 °C
		83 kW	1200 °C
Natural convection	Nitrogen	20 kW	± 460 °C
		60 kW	975 °C
		85.5 kW	1200 °C
Near-vacuum (10kPa-g)	Nitrogen	20 kW	580 °C
		82.7 kW	1200 °C

The power supply of the experiment had the capacity to drive the heating elements at over 250 kW. The feasibility of extending the tests to reach temperatures of up to 1600 °C was investigated but never completed.

In Chapter 5 the results from the Isothermal Flow measurements and in Chapter 6 selective results from the forced convective tests will be presented. In the case of the numerical models, the forced convection case of 140 kW and 1 kg/s was used to calibrate the model. Other cases considered in comparison only

are for a heater power of 140 kW at 0.5 kg/s and 2 kg/s as well as the 120 kW-case with gas flow rate of 1 kg/s. Comparison with the natural convection and vacuum tests are not included in the scope of this study, as this has been covered extensively in the past through work on the effective thermal conductivity (Van Antwerpen, 2009), (De Beer, 2021); and corresponding radiation models (Pitso, 2011), (Van der Walt, 2020).

4.2.4. Description of the Facility

This sub-section outlines the relevant information regarding the HTTU as applicable to the numerical modelling of the relevant experiments.

Physical Description

The HTTU consisted of a main pressure vessel connected to four parallel flow circuits consisting of heat exchangers, blowers and piping. The internal structure contained a central heating element embedded in a graphite cylinder, insulated ceramic base with flow channels, surrounded by an outer graphite reflector forming an annulus to contain spherical graphite balls – the annular pebble bed. The outer reflector was continuously cooled by a water jacket and coolant gas was blown from below from the four parallel circuits. In each, heat was removed by water-cooled shell-in-tube heat exchangers. Detail of the facility and vessel internals are shown in Figure 4.1 below.

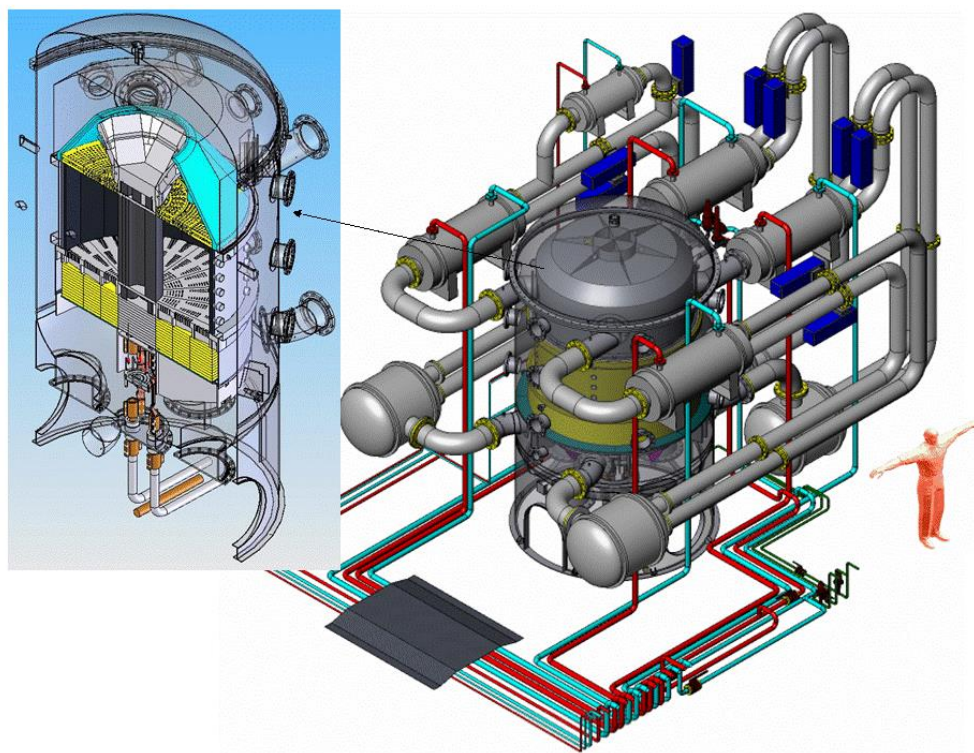


Figure 4.1: A 3D rendering of the HTTU test bed internals (left) and the full assembly (right) with person for scale (Rousseau & Van Staden, 2008).

Altitude

The HTTU was located in Potchefstroom, South Africa at an altitude of 1350 m above MSL which corresponds to an absolute air pressure of 86.4 kPa and it is presumed that the experiment was operated during forced convection tests at a pressure slightly above ambient to avoid air (oxygen) ingress. In all cases where applicable, an absolute pressure of 90 kPa (corresponding to a gauge pressure of 3.6 kPa) was applied in modelling. This could not be verified from available measurements in the documents to which access was provided.

4.3. Model Set-Up

This section describes the inputs and parameters used to obtain the results presented in Chapter 7 in sufficient detail. Where further input, values or functions would be necessary, a concerted effort has been made to provide these in Appendix B of the document.

4.3.1. Computer Code

In both numerical cases described, the commercial CFD code *Siemens Simcenter Star-CCM+* (Siemens, 2023) was used. All the inputs and results described or shown visually in this study, have been realised using Version 2310.0001 (18.06.007) of the single precision version of the code, the latter in order to minimise memory usage. The North-West University is an academic license holder of the software and the author has made use of the POD (power-on-demand) function from the pool of hours belonging to the NWU.

4.3.2. Hardware

The majority of simulations were done on recent professional workstation-grade hardware. The details of the primary calculation computer are provided below:

- Dell Precision T7920 workstation
 - CPU: 2x Intel Xeon Gold 6136 12-core 3.00 GHz 3.7 GHz Turbo
 - RAM: 192 GB 6-channel DDR4-2666
 - I/O Drive: 2TB NVMe SSD
 - GPU: NVIDIA Quadro RTX 4000 8 GB (not used for solving)

Additionally, the North-West University provides access to its own high performance computing cluster, the NWU-HPC which is capable of solving scalable CFD problems in parallel. Due to the focus of a robust and middle-resolution model, the HPC was used for initial mesh dependence studies early in the study.

CHPC

The Centre for High Performance Computing (CHPC) forms part of the South African National Integrated Cyber Infrastructure System (NICIS) and is funded by the Department of Science and Innovation. It is one of the objectives of this infrastructure to promote the development of science and industry by making high-performance computing available to public non-commercial interests such as academia, without cost.

The CHPC was utilised for final mesh dependence verification as well as for additional parametric runs of higher and lower power cases, where repeatability was needed. It is a future prospect to investigate much finer mesh resolutions in order to understand the numerical dependencies but falls outside the scope of this study which aims to present a model that does not depend on high-performance computing.

As required by the academic agreement with the NICIS CHPC, the author acknowledges the Centre for High Performance Computing (CHPC), South Africa, for providing computational resources to this research project.

4.3.3. Budgetary remarks

The discipline of this study is that of Nuclear Engineering, and not science or thermo-fluid physics *per se*. A remark must therefore be made on the feasibility of both model robustness (accuracy and reliability) and computational effort on hardware that would be accessible to a vendor or design house applying a numerical model in order for design validation or safety analyses of a pebble bed reactor design. There are two competing forces at play, as shown in Figure 2.14: that of level of detail versus that of computational time.

There are three aspects to the financial implications in the use of commercial numerical codes in nuclear engineering analyses:

- Licensing costs
- Hardware costs, either through purchase and rental or CPU-time
- Human resource costs

A CFD model with a high level of detail is costly in terms of solution time, and would therefore be scaled to more powerful hardware. With this scaling comes an increase in the license demand as well, leading to an increase in overall financial cost. In most cases it would be assumed that access to or use of high-performance supercomputing hardware would lead to unnecessary cost versus the value of the output,

although in the experience of the author several vendors, research partners and universities do own computer clusters and contribute to analyses in terms of numerical simulation.

As a general rule then: if the objectives of a numerical analysis are to be met, the model used must show acceptable accuracy with reasonable computational requirements (i.e. practically achievable within project timeline and budget).

It is to satisfy this requirement, then, that the efforts of this study were focussed on realising a validated numerical model with acceptable accuracy, capable of running on workstation-grade hardware within a reasonable timeframe (several days to a week per run).

4.3.4. Geometry

For the discrete approach, an explicit geometry generated by DEM, as described in Chapter 3, was used for the solid domain described in the CFD model. The fluid domain was extracted as a binary subtraction from that of the solid volume.

For the porous approach the porosity distribution as analysed from the DEM positional data was used, with the domain discretised in several axial and radial sections and the corresponding average porosity from the analysis, applied to each.

Three levels of detail were considered for the study:

- Pressure vessel internals
- Bed inlet and outlet
- A section of the bed

Initially, a full-scale simulation of all the pressure vessel internals was done using a porous medium to model the bed. The objective of this was to determine the symmetry of flow within the vessel and of that reaching the bed. It was found that the flow reaching the bottom of the bed was distributed equally and that symmetry about the planes parallel to the x -axis and y -axis may be assumed.

The bottom support of the HTTU internal structure, supporting the pebble bed as well as allowing gas to enter the bed, is divided into 16 sections with identical geometry. This led to the further simplification of using a 1/8th geometry for further testing, before heat transfer models and in particular, surface-to-surface radiation, were included.

Ultimately, the 1/16th symmetrical section geometry as shown in Figure 4.2 was selected as this allowed the necessary fine mesh and refinements to be done on a workstation and allowed sufficient RAM allocation for the surface-to-surface heat transfer model.

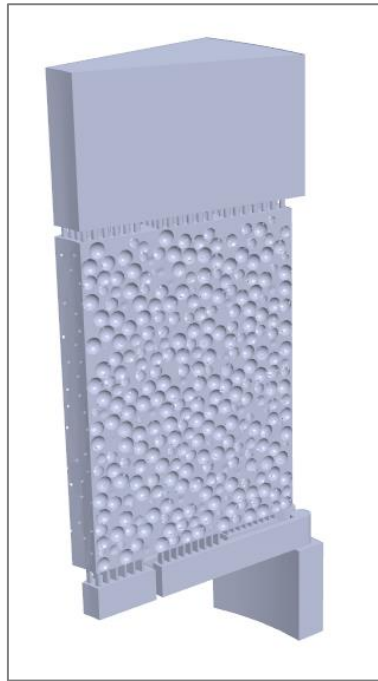


Figure 4.2: 3D view of the 1/16th geometry used for the fluid domain in the discrete geometry approach.

Several smaller geometries that were taken from sections of the bulk region were used to calibrate the surface-to-surface radiation model parameters.

4.3.5. Mesh

In their work on CFD applied to packed columns of various fill shapes in the chemical industry, Jurtz *et al.* (2019) discussed various mesh types and the importance of local geometric modifications, especially in the vicinity of contacts.

Because of the optimised use of volume-to-cell-count ratio of polyhedral cells, the advanced polyhedral meshing method implemented in Star-CCM+ was applied in this study in order to minimise cell count whilst achieving acceptable mesh quality. This aspect is only relevant to the discrete approach and the local mesh refinement is discussed in further detail below.

4.3.5.1. Discrete Approach

The prominent geometric features and details that require sufficient definition in the mesh are:

- Gaps around pebble-pebble and pebble-wall contacts
- The inlet manifold and flow paths into the bed
- The boundary layers on solid interfaces

In selecting and testing mesh parameters, these features were considered and the skewness of cells checked in their vicinity. In Table 4.3 below the mesh parameters selected for the final discrete geometry model is shown.

Table 4.3: Mesh parameters of the discrete geometry approach.

Mesh property	Value
Base size	8.0 mm
Number of boundary layer cells	3
Boundary layer stretching	1.4
Boundary layer thickness	2.64 mm
Target surface size	20 mm
Minimum surface size	1.2 mm

A part of the resulting mesh is shown in Figure 4.3 for the fluid domain around pebbles, for pebble-pebble and pebble-wall contacts as well as the solid domain of the inner reflector (left). In tests with more boundary cells on the heater surface it was found not to have a significant effect on the heat transfer or temperatures.

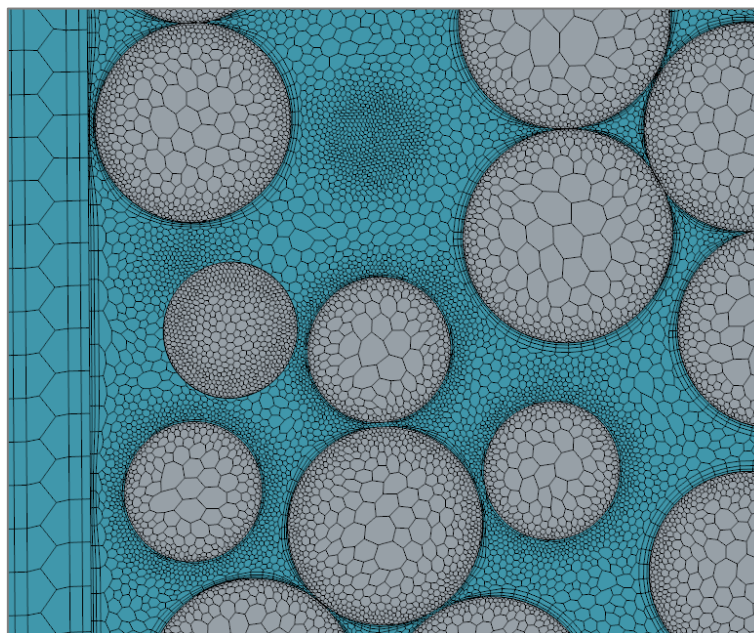


Figure 4.3: Close-up of the polyhedral mesh as seen on a symmetry plane for the discrete pebble model.

In Figure 4.4 further detail of the resulting mesh of the fluid domain on the bottom and around the inlet manifold and tubes is shown. As can be seen, sharp corners on the inlets were left as-is, as this reduced mesh count and the flow velocity is relatively low here compared to between spheres, for example.

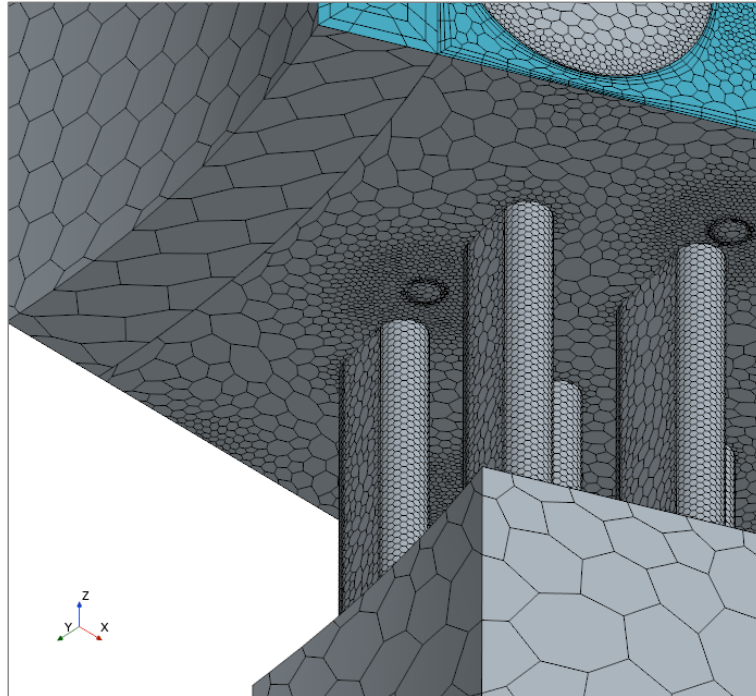


Figure 4.4: Close-up detail of the resulting polyhedral mesh of the flow domain around the manifold and inlet tubes on the bottom of the bed.

In a comparable study done using the same CFD code on a section of the cylindrical core and riser tubes of the Xe-100, Van Staden *et al.* (2018) used similar values for minimum size and boundary layer thickness and stretching, but used 8 layers for boundary cells and a base size of 20 mm. It is suspected that this is what was necessary to accurately model the heat transfer from fuel pebbles containing a source of heat.

4.3.5.2. Porous Approach

A porous medium representation is seen as a coarse mesh method. In the case of the porous approach, the mesh fineness was chosen to have sufficient resolution in order to capture the varying porosity as prescribed (see Figure 4.5 below) as well as the boundary layer in the wall regions, thereby capturing the resulting changes in other dependent (solved) parameters such as velocity.

With a significantly lower mesh count and memory requirement compared to the discrete geometry approach, it was not necessary to consider symmetry or only a section of bed and the entire bed could be modelled.

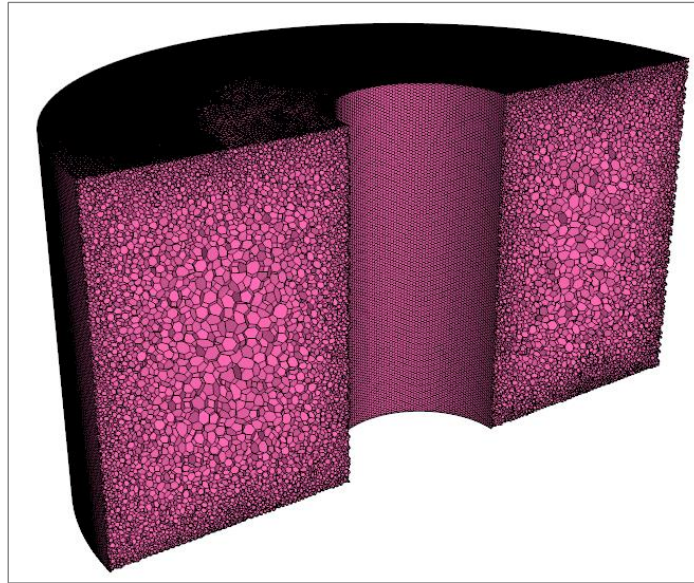


Figure 4.5: A 3D view of the porous approach mesh, showing refinements near the walls and inlet and outlet surfaces.

4.3.6. Boundary conditions and physics parameters

In both approaches, the same boundary and initial conditions were applied under which the experiment was operated. As will be discussed in the next section, both the heat input and mass flow rate were ramped up from zero in order to promote numerical stability.

Heat input

Due to the presence of stem coolers underneath the heater elements as well as conduction losses through the support structure, a parasitic load of 8 kW is prescribed for the primary case of 140 kW as determined from records of the experiment. Therefore, the heat input that was applied is set up as a fixed heat input of 132 kW on the heater-side surface of the inner reflector. The assumption of a constant flux over the inner area is also deemed an appropriate choice, given the encased graphite structure of the heater assembly. As the geometry that was considered is a 1/16th section, the actual value of heat input was entered as 8 250 W.

Mass flow

The mass flow rate and temperature of the inlet gas stream was set as 1 kg/s and 40 °C, respectively. In the experiment, the outlet gas cooling system was set to control the inlet at this temperature and the blowers were calibrated in order to achieve this mass flow at the inlet temperature. Once again 1/16th of the value was entered as 0.0625 kg/s, due to the sectional geometry considered.

Turbulence modelling

The Navier-Stokes equations for mass, momentum and energy conservation as embodied in Star-CCM+ were solved numerically in the simulations. It was discussed in Section 2.4.3 that various authors have shown acceptable results using RANS turbulence modelling.

Therefore, a RANS approximation with a Realisable k - ε Two-layer all y^+ wall treatment was selected to model turbulence. As the fluid is a real gas at a temperature and pressure easily representable as an ideal gas without any special considerations, the default values for the coefficients associated with this turbulence model, were used. For the mass flow inlet used, the turbulence intensity and viscosity ratio were set to 0.01 and 10, respectively.

4.3.6.1. Discrete approach

Pebble thermal contact resistance

A drawback of a static geometry (not coupled with a soft body DEM model) means that the pebble contacts are not dynamic with regards to thermal expansion, movement and compression of the spherical bodies. For this reason, in the discrete model, the contacts between pebbles are defined but not resolved based on their geometry alone. A user function was defined to describe the thermal contact resistance and the model used was that of De Beer (2021). This configuration is mentioned here as it forms part of the geometry and mesh workflow to identify contacts in the solid domain.

Radiation

To account for internal radiation in the fluid medium, grey thermal surface-to-surface radiation with ray tracing view factors (one surface to many surfaces) calculator was chosen. The emissivity of all surfaces was chosen as 0.8 as this value is commonly agreed as the appropriate. Due to the close proximity of similar material surfaces this was not optimised and later results did not give reason to reconsider the selected method and values.

4.3.6.2. Porous approach

Effective thermal conductivity

To account for radiation, the model for thermal conductivity of Ren *et al.* (2017) was implemented (see Appendix B) as it was determined from the TF-PBEC facility and may be considered the most up to date from literature.

4.3.7. User Functions

The software allows users to define expressions using mathematical and logic operators in Java to be included during solving. The parameters that may be defined by the user includes thermophysical properties, boundary conditions and correlations for coefficients present in physics models.

Discrete Approach

The following user defined functions (UDFs) have been defined and used in the CFD model and the full definitions and code may be found Appendix B:

- i) The inner and outer reflector graphite thermal conductivity (Appendix C, from *UCAR*) as a function of temperature in Kelvin.
- ii) The pebble thermal conductivity (Appendix C, from *SGL*) as a function of temperature.
- iii) The contact resistance between pebbles, as a function of temperature (De Beer, 2021).
- iv) The nitrogen density is prescribed as a real gas according to the Van der Waals equation of state.
- v) Nitrogen specific heat from the general formulation for an ideal gas.
- vi) Nitrogen dynamic viscosity (Kleiber & Joh, 2010).
- vii) Nitrogen thermal conductivity (Kleiber & Joh, 2010).
- viii) Nitrogen turbulent Prandtl number (from definition of the dimensionless number).
- ix) A ramp of the steady-state inlet mass flow boundary condition as a function of the iteration number (for numerical stability and convergence reasons).

Porous Approach

In the porous approach implemented in Star-CCM+, the porous viscous and inertial terms need to be defined according to Darcy's law (Siemens, 2023). This is easily done for any Darcy-type pressure loss correlation. As the correlations depend on porosity, this has been included as a variable in the UDF. The formulation used is provided in Appendix B-2 and the values taken from Table 3.6.

Figure 4.6 shows the porosity distribution assigned to different regions in the bed, also defined by a UDF.

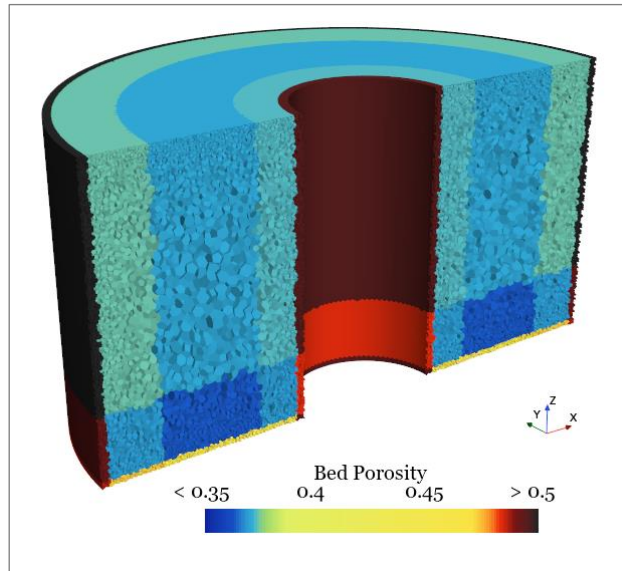


Figure 4.6: 3D view of the coarse mesh porous medium geometry with the colour scale indicating porosity as defined in a user-defined function dependent on radius and height.

4.3.8. Code Execution

The solver was only run in steady-state with disabled physics for heat transfer initially, including radiation, in order to significantly reduce CPU time. If the mass and heat inputs are not gradually ramped up with the defined user functions, the solution was unstable and failed.

Firstly, the segregated energy solver was disabled for the first 1 000 iterations and the density of the nitrogen phase was defined as a compressible ideal gas. After this initial period where the flow was allowed to develop the energy solver was enabled and the heat input was ramped up and here the gas was changed to a real gas with Van der Waals equation of state. The target value of mass flow rate was reached at 4 500 iterations and after 8 500 iterations the full input energy was reached. It was only at this point that the surface-to-surface radiation heat transfer solver was enabled and overall convergence was reached before 12 000 iterations.

In this way it was possible to automate the changes by using user-defined functions and macros when setting up the simulation, so that it could be run to convergence without requiring user input. This functionality is also possible when submitting the simulation to a remote queue as an HPC job.

4.4. Chapter Summary

In this Chapter the set-up and execution of both porous and discrete geometry approaches in the CFD software was discussed. Details were provided particularly on mesh setting as well as configuration of parameters essential to the modelling of pebble beds: the contact resistance, in the case of the discrete geometry approach, and the effective thermal conductivity in the porous semi-analytical approach.

In the following chapters the experimental results from the HTTU facility are discussed. Measurements from the isothermal forced flow case are discussed in Chapter 5 with some images from the CFD of the equivalent simulation, in order to better visualise the conditions that could have given rise to the measurements.

End of Chapter



5. ISOTHERMAL TESTS

This Chapter discusses the isothermal tests and the associated numerical models, presenting the velocity measurements obtained from the HTTU experimental campaign with isothermal forced flow in nitrogen.

The data has been obtained from M-Tech Industrial (Pty) Ltd. (2009a) and has been used with permission from PBMR® Pebble Bed Modular Reactor SOC Ltd. (2016).

The tests were done with a gas inlet temperature of 18 °C and the pressure is not known. As described in Section 4.2.4, the absolute pressure will be assumed to be 90 kPa if no other information is available.

5.1. Flow and Pressure Drop Characteristics

KTA 3102 Part 3 (1981) prescribes a Darcy-type friction factor as a function of the modified Reynolds number as is commonly applied to packed beds.

Substituting the values for the isothermal test at 1 kg/s into the KTA equation (see Appendix D), the pressure drop predicted by the correlation for this test is $\Delta p_{\psi} = 23.1$ Pa.

Gas mass flow rate

Sub-dividing the cross-flow area into radial increments corresponding to the radial positions of the measurement locations and calculating the area of the increments using half an increment to the inside and half an increment to the outside, it is possible to use area, measured velocity and gas density to determine the average mass flow of that increment. As the test was specified to have been done at a certain total mass flow rate, this should correspond to the total over all the increments considered. This was found to not have been the case, however, and a correction has been applied in order to reach a total of the correct mass flow rate when summing over all radial increments.

5.1.1. Velocity measurements

In order to conduct velocity measurements, a tangentially and radially traversing armature with hot-wire measuring probe was placed above the annular packed bed, but within the pressure vessel, thereby opening the normally enclosed space between the top of the bed and the pressure vessel walls (M-Tech Industrial, 2009a). Velocities were measured along three radial lines, 120° apart, and at 47 measurement points with finer incremental distance closer to the respective wall boundaries.

The results presented are the averaged velocity measurements with uncertainty at the radii indicated, taken at 60 mm in Figure 5.1 and 75 mm above the bed in Figure 5.2, both normalised to 1 kg/s.

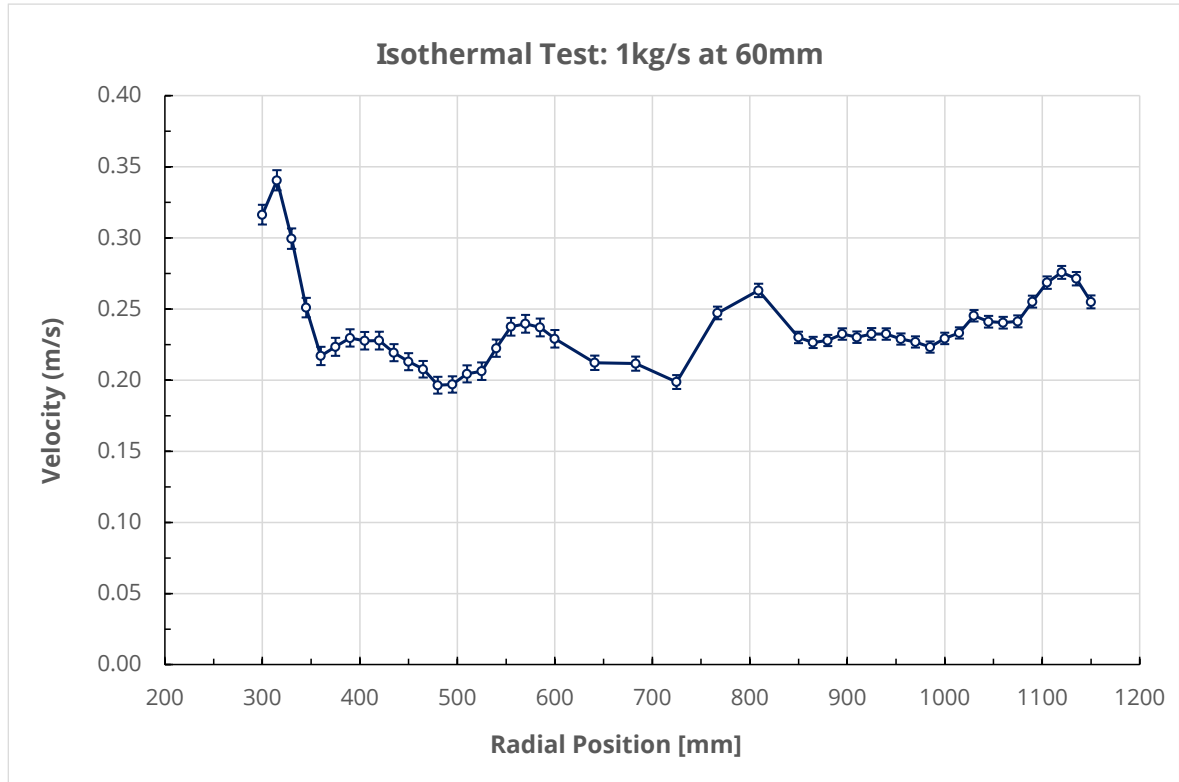


Figure 5.1: Average velocity measurements 60 mm above the bed for the 1 kg/s forced flow isothermal case.

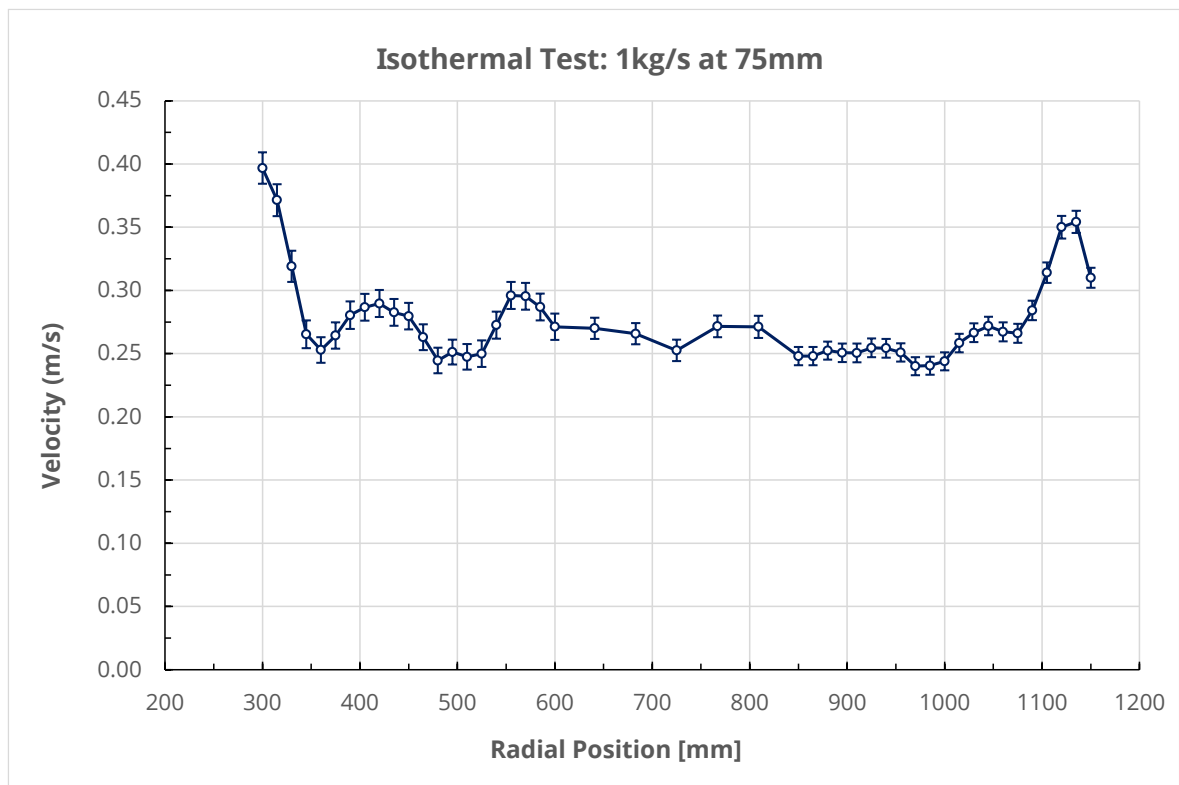


Figure 5.2: Average velocity measurements 75 mm above the bed for the 1 kg/s forced flow isothermal case.

5.1.2. Observations from the CFD model

Pressure losses

In the discrete CFD simulation, the pressure loss through the 1.2 m height of the packed bed is calculated as 21 Pa and the overall pressure drop (including inlet manifold and volume above the bed) as 42 kPa. The pressure drop predicted by the analytical approach is in good agreement with the corresponding pressure drop over the 1.2 m height of the bed obtained by the CFD simulation. As no pressure drop measurements are reported on in the HTTU isothermal test report (M-Tech Industrial, 2009a), no conclusion can therefore be drawn on the validity of the modelled overall pressure drop.

The static pressure distribution obtained in the CFD of the discrete geometry is shown in Figure 5.3 below.

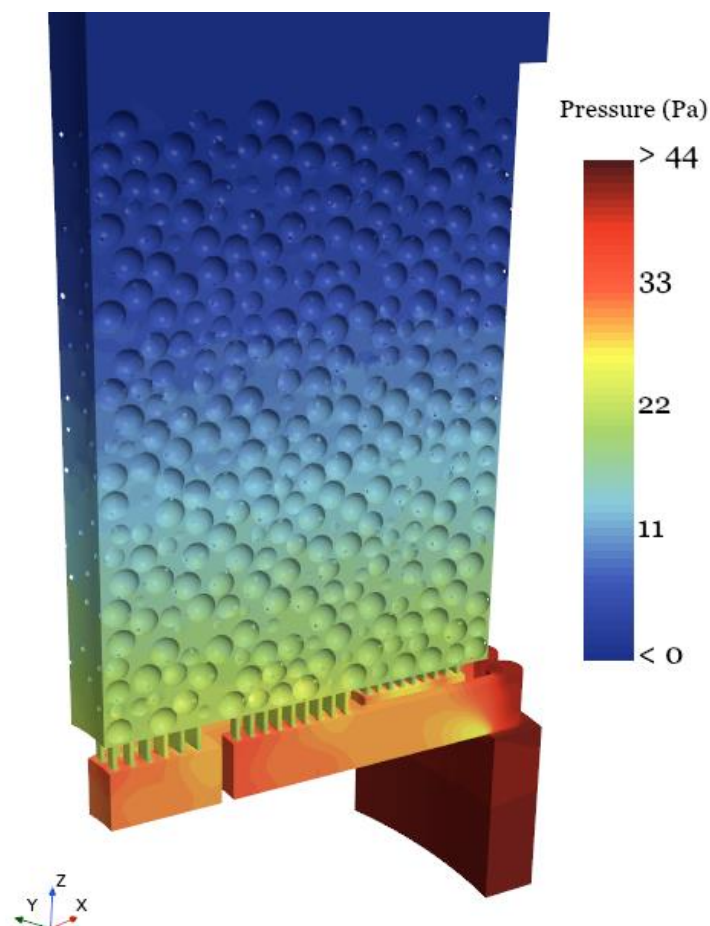


Figure 5.3: The relative pressure distribution in the discrete CFD approach 1 kg/s isothermal case.

Velocity Distribution

In the velocity measurements shown in Figure 5.1 and Figure 5.2 it is observed that there are several peaks in velocity values, in particular near the inner reflector and also, yet to a lesser degree, near the outer reflector wall as several smaller peaks. These observations are expected, due to the wall channelling effects shown in Figure 2.2 and discussed in Section 2.1.4.

Looking at the velocity distribution along the x -plane from the CFD results shown in Figure 5.4, the presence of higher-than-average velocity plumes are seen, along the bed, but especially in the vicinity of the inner and outer reflector walls.

The velocities shown in Figure 5.4 are localised values, and to make a meaningful comparison with the averaged results as shown in Figure 5.1 and Figure 5.2, the velocities in the xy -planes at the relevant axial positions need to be obtained. This is discussed further in Chapter 7.

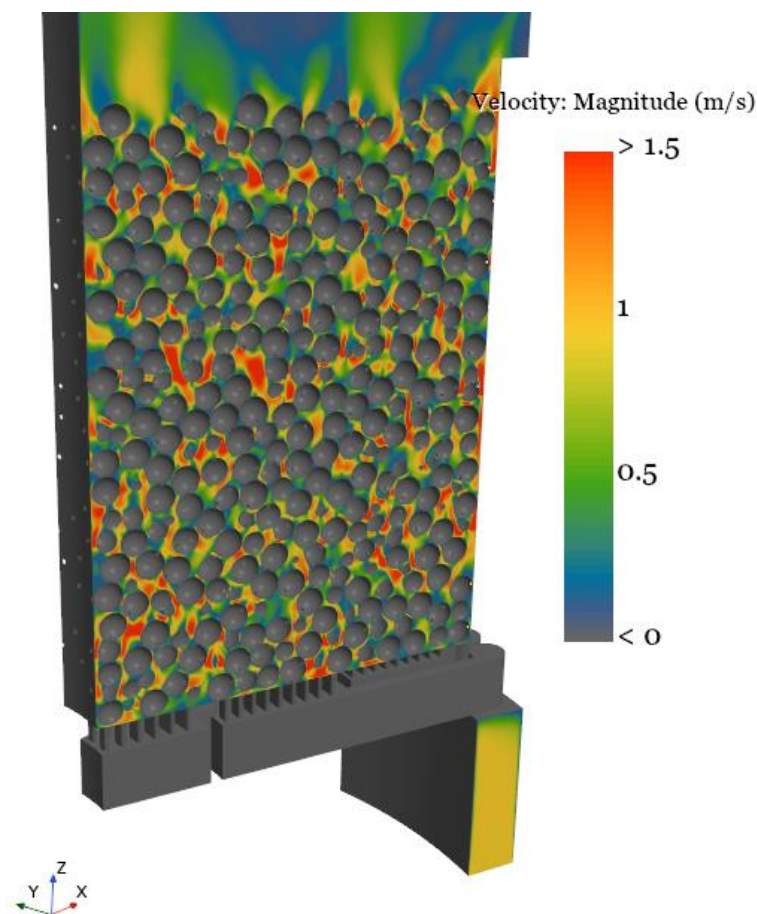


Figure 5.4: Velocity distribution in the discrete CFD approach 1 kg/s isothermal case.

It is also important to keep in mind that the exact packing configuration of the spheres under each of the radial lines considered in the experiment, is unknown. No observations can therefore be made regarding the correspondence or not between the experimental and the numerical packing configurations and their effect on the velocities obtained.

Flow mixing

The mixing or *braiding* of flow is another characteristic of pebble beds. Velocity streamlines from the discrete approach CFD results for the 1 kg/s isothermal case is shown in Figure 5.5 below. Here it is clear that the characteristic length or flow path is a significant factor and not only the pebble diameters.

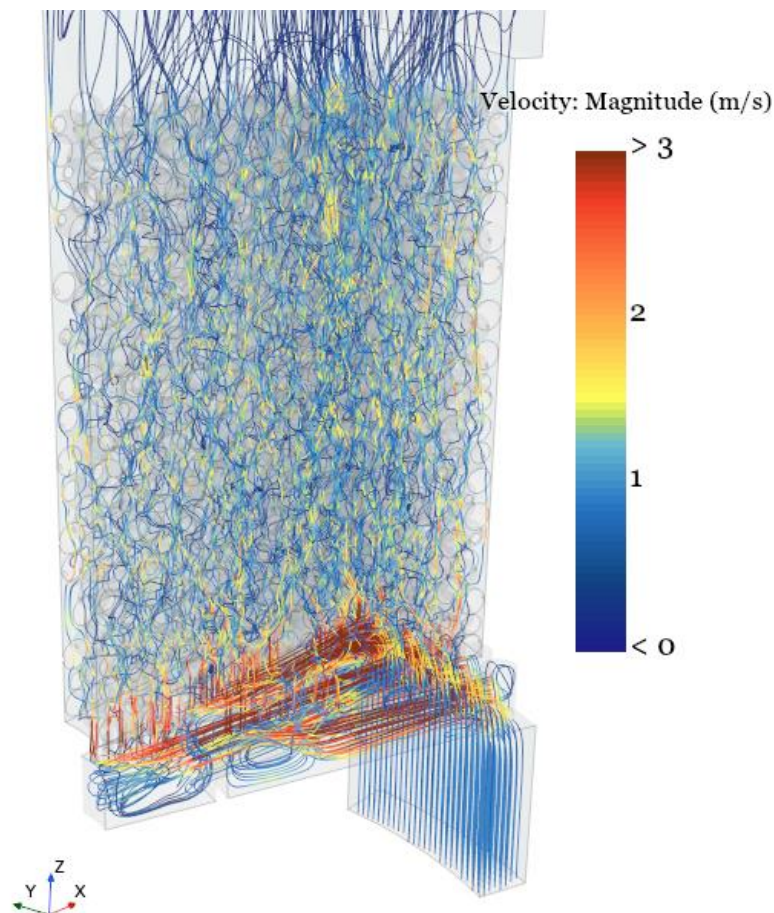


Figure 5.5: Velocity streamlines (colour indicates magnitude) in the discrete CFD approach 1 kg/s isothermal case.

The streamlines originate at the inlet at equally spaced points. Considering that the geometry is a section and 'wedge'-shaped if viewed from above, it can be concluded that the flow distributes fairly uniformly and that wall-channelling affects primarily the velocity magnitude and not flow distribution.

Figure 5.6 shows a scalar field plot of the gas velocity magnitude for the isothermal case as solved by the porous model. It may be observed how the porous approach homogenises the flow in all but the near-wall regions. The velocity is mostly dependent on the porosity in this formulation and details of local flow effects are lost.

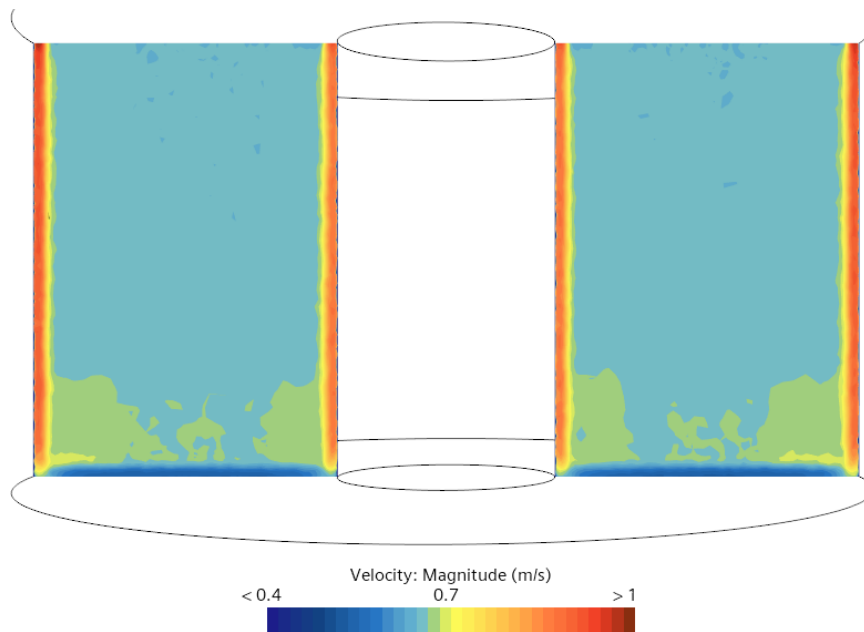


Figure 5.6: Scalar field plot on a planar surface through the centre of the porous model bed of the gas velocity magnitude.

5.2. Chapter Conclusion

In this Chapter the experimental velocities measured during isothermal test were presented. Some preliminary results of the velocity distribution obtained in the CFD simulation have also been shown. A detailed comparison between the measured experimental velocities and the calculated numerical velocities will be presented in Chapter 7.

End of Chapter

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6. FORCED CONVECTION TESTS

This chapter focusses on the heat transfer aspects of the HTTU tests. The results obtained from the HTTU experimental campaign with forced convective heat transfer in nitrogen is presented and discussed at the hand of the associated numerical models.

The data has been obtained from M-Tech Industrial (Pty) Ltd. Reference (2009d) and has been used with permission from PBMR® Pebble Bed Modular Reactor SOC Ltd. (2016).

The tests were done with a gas inlet temperature of 40 °C and various mass flow rates and thermal heater powers. Similarly to the isothermal case, the pressure is not known and assumed to be 90 kPa.

6.1. Measurement Points

The placement of thermocouples and other elements in the HTTU forced convention tests are shown in Figure 6.1. For the tests during preparation and packing of the bed, instrumented pebbles were placed in a line all in contact with the adjacent pebbles or walls at the ends.

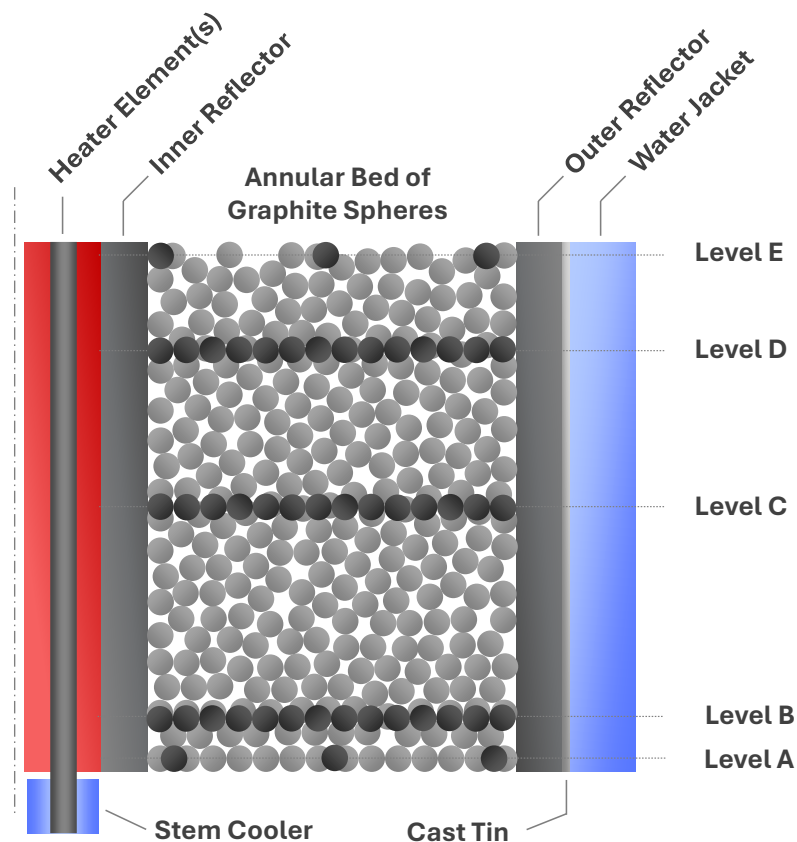


Figure 6.1: Components of the HTTU annular unstructured bed experiment with instrumented pebbles shown.

When viewed from the top, three radial lines of these rows were placed 120° apart and on three different levels, for a total of 9 such instrumented pebble rows. The thermocouples on Levels A and E are not considered for comparison and were not reported in (M-Tech Industrial, 2009d) as they were used for control measurements.

The outer reflectors consisted of 24 flat graphite plates at a radial distance as shown in Figure 6.2. As their circular assembly does not form a tight contact with the circular water jacketed, molten tin was cast into the gap (NWU, 2009). This was considered as a separate solid material region in the simulation.

In Figure 6.2 the locations of the thermocouple positions with associated uncertainty are shown to scale. The same positions in terms of height were used for temperature probe lines in the solid domain of the CFD. In the porous approach the same tangential locations were used with finer increments.

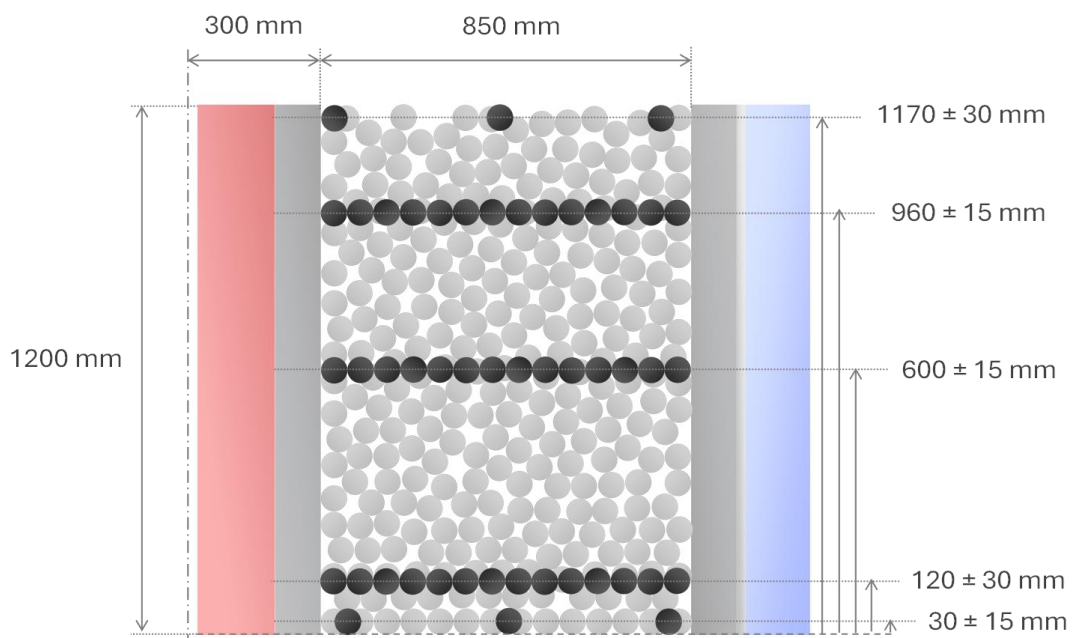


Figure 6.2: Location of thermocouples (in black) placed in the forced convection tests (along 3 radial lines at different heights at 3 tangential positions).

Discrete approach

In the discrete geometry approach that modelled a smaller 1/16th section of the entire bed, more tangential lines were placed as shown in Figure 6.3. During the DEM generation of the packed bed no spheres were packed in radial lines corresponding to the instrumented radial lines in the experiment.

For the temperature measurements in the discrete geometry model the *line probe derived part* was used. The placement of these probe lines is shown in Figure 6.3 each with a resolution of 100 unique measurement points. If the point corresponds to a cell in the solid domain, the value of that cell was extracted. For the axial placement, the same height as that of the experiment was used, the values shown in Figure 6.2 above.

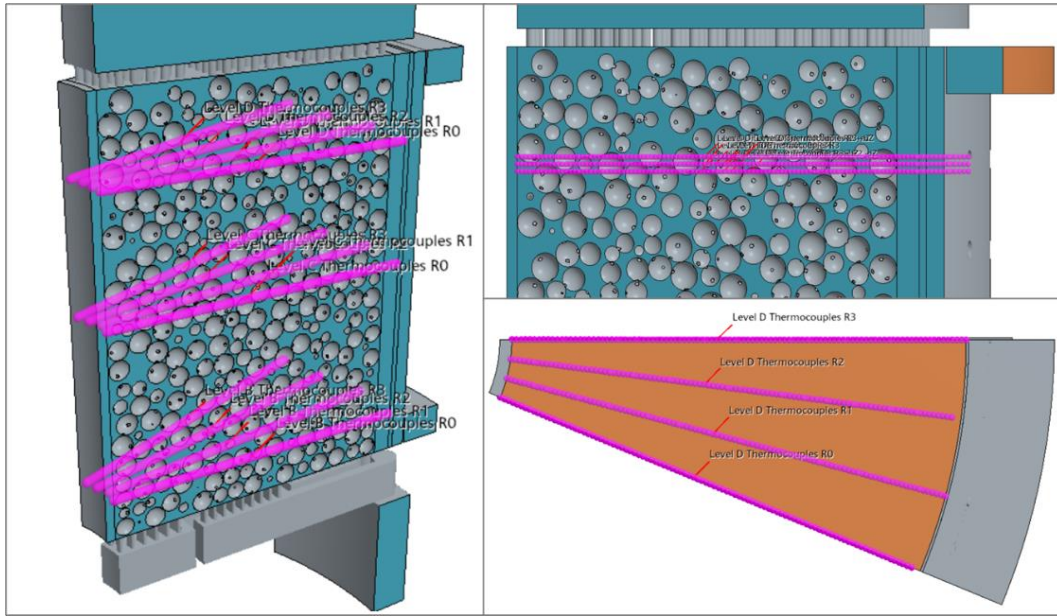


Figure 6.3: Isometric (left), side (top right) and top (bottom right) views of the different line probe placements in the discrete geometry model to represent measurement points in the experiment.

Additionally, two more lines were placed at a distance of $+dz$ and $-dz$ above and below the probe line of each level on the z -axis, with dz corresponding to the uncertainty of axial position as shown in Figure 6.2 (± 15 mm for Level D, for example).

Due to the discrete geometry and porous structure being explicitly defined, it was necessary to place more tangential probe lines around the vertical z -axis. Therefore, on each level, four probe lines were placed tangentially 7.5° apart. The outermost lines corresponded to values on each of the respective symmetry planes, with two lines in the volume in-between.

The measurements from each of the additional axial and tangential on a line corresponding to the same radial points were averaged, and the standard deviation calculated.

Porous approach

In the porous approach, the same *probe line derived part* was used to extract measurements. The same three levels and three tangential lines were used as done in the experiment. Due to the porous medium defining a solid temperature in each cell that was probed, a fewer number of measurement points were necessary per probe line and the same number of points as in the experiment was used in the simulation. At the inner and outer reflector walls, one point was placed in the solid wall and another close by in the porous domain. The probe lines that were used are shown in Figure 6.4 below.

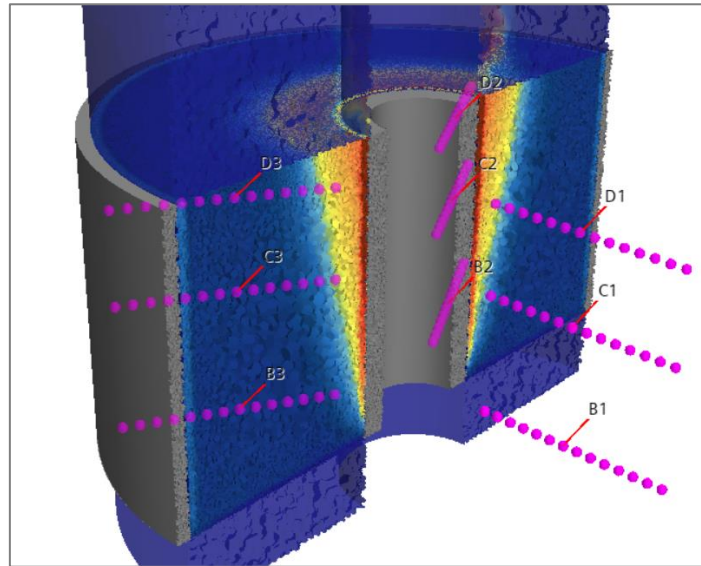


Figure 6.4: Isometric view of the different line probe placements within the porous medium model to replicate measurement points in the experiment.

6.2. Porous Approach

6.2.1. Heat Transfer Phenomena

Section 2.1.5 previously discussed the different heat transfer phenomena in pebble beds, as shown in Figure 2.3. It is expected that in both the porous and discrete geometry approaches, the porous structure and therefore porosity will be a driving factor in many of the flow and heat transfer parameters.

6.2.2. Correlated Parameters in the Porous Approach

As discussed in Section 4.3.6.2 the porous approach relies on UDFs to define the required material properties and flow and heat transfer parameters associated with a porous medium model. For these inputs the KTA correlations as defined in Appendix D were used in the Java script form as shown in Appendix B.

Values of the KTA correlation parameters

The porosity as determined from the methods described in Chapter 3 and previously shown in Figure 4.6 is again included as Figure 6.5 (a) for reference as well as the velocity magnitude calculated by the code in (b) for the porous approach. The other values related to the thermal-hydraulics are: the modified Reynolds number Re_m in c), effective thermal conduction k_{eff} in d), pebble-coolant convective heat transfer coefficient α in e), and the correlated Nusselt number Nu_{KTA} in f).

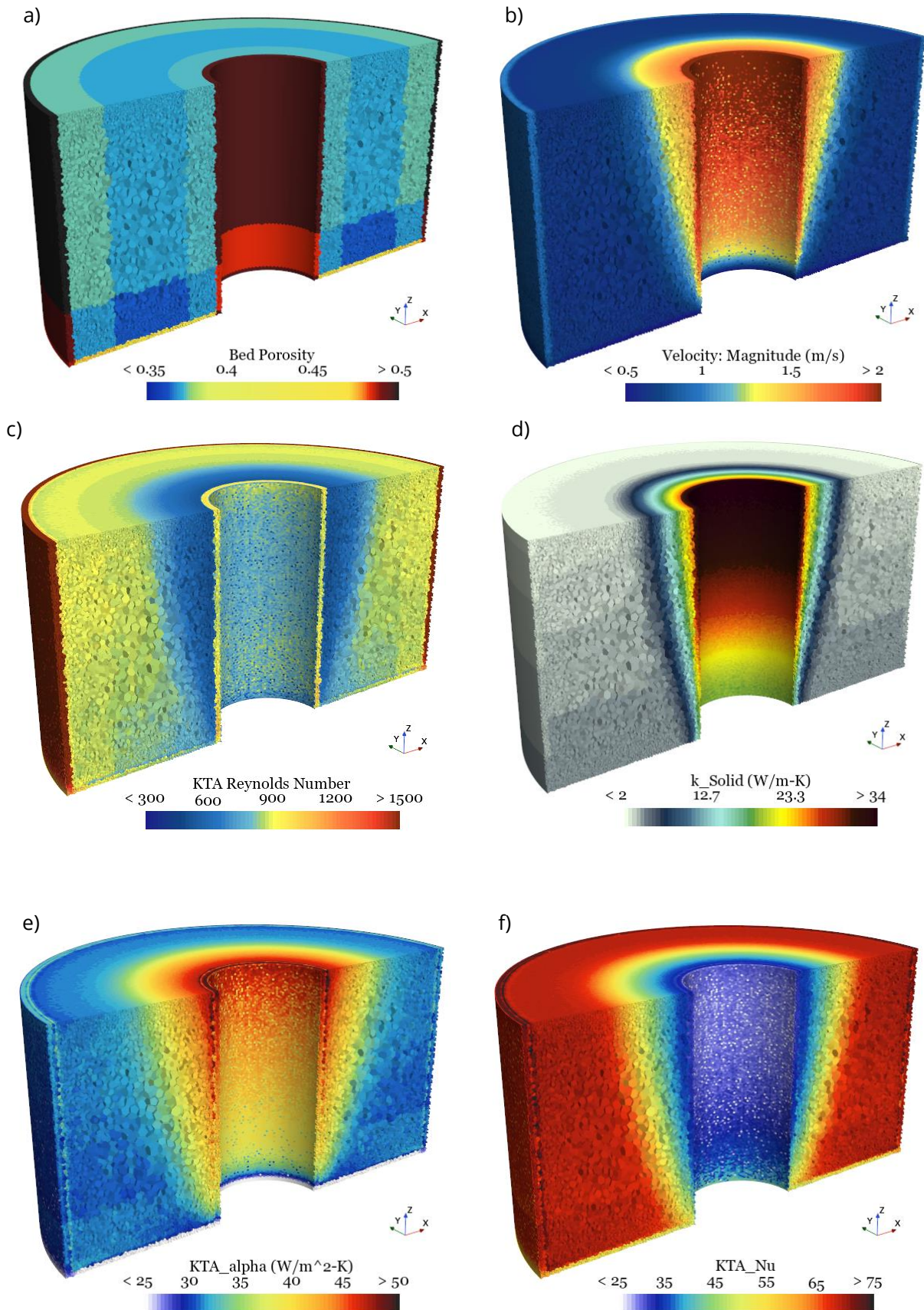


Figure 6.5: Values for several calculated values or UDF correlations from the KTA standards in the porous approach: a) porosity, b) velocity, c) modified Reynolds number, d) solid conductivity, e) convection coefficient and f) Nusselt number.

It can be seen in Figure 6.5 (a) to (f) that the correlated values are influenced strongly by the velocity through the modified Reynolds number and also the porosity.

Temperature Results

In Figure 6.6 below the calculated temperature for a) the solid and b) the gas phases of the porous model are shown. The temperature distributions are similar with a clear upwards shift in that of the gas phase due to convective heating.

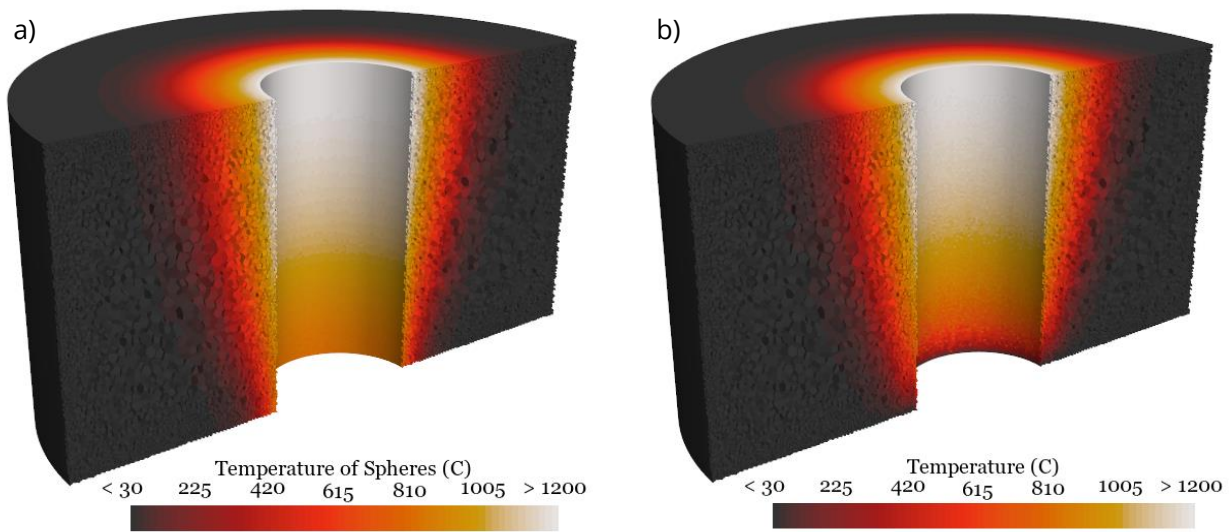


Figure 6.6: Temperature results of the a) solid and b) fluid domain of the porous model.

The relevant velocity and temperature profiles were extracted from these numerical results in order to be compared with the corresponding experimentally measured values. The results are presented and discussed in Chapter 7.

6.3. Discrete Approach

The intent of the discrete geometry model was to resolve as much of the geometry and physics of the HTTU under forced convection as practical numerically. The necessary modelling of turbulence and sphere-sphere contacts has been discussed in Section 4.3.6 along with suitable mesh parameters.

In Figure 6.7 (a) the velocity results are shown on the symmetry plane (with solid domain in grey) as calculated in the numerical model using a discrete geometry for the benchmark forced convection case of 1 kg/s with 140 kW heating. Similarly, the temperature distribution in both solid and fluid domains is shown in Figure 6.7 (b) and it is from this that the corresponding data was extracted.

It is noteworthy to consider the relatively high local velocities close to the inner heated reflector showing a clear influence on the gas flow by temperature dependent density and viscosity property values. This, together with the lower physical porosity in the near-wall region, contributes to the observed velocity.

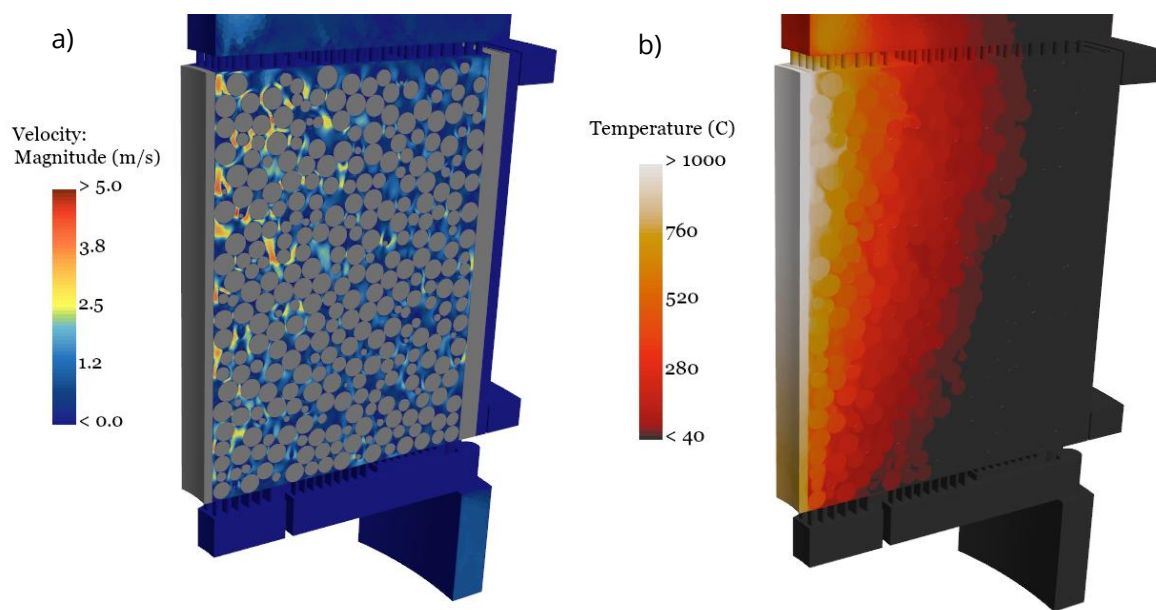


Figure 6.7: Numerical results of a) velocity and b) temperature of the 140 kW heated 1 kg/s forced convection case using the discrete geometry approach.

The final qualitative results of both approaches are presented in the next Chapter in graph form as comparison to the corresponding experimental measurements.

6.4. Measured Temperatures

The forced convection tests at a power level of 140 kW were performed three times (M-Tech Industrial, 2009d). The average value for each point across all tests are shown in Figure 6.8 as the dotted blue line. The second test values are shown as the orange line, labelled “recommended”. Due to problems with the particular thermocouple in the location around 0.54 to 0.6 m on Level B, this value is removed from the latter dataset.

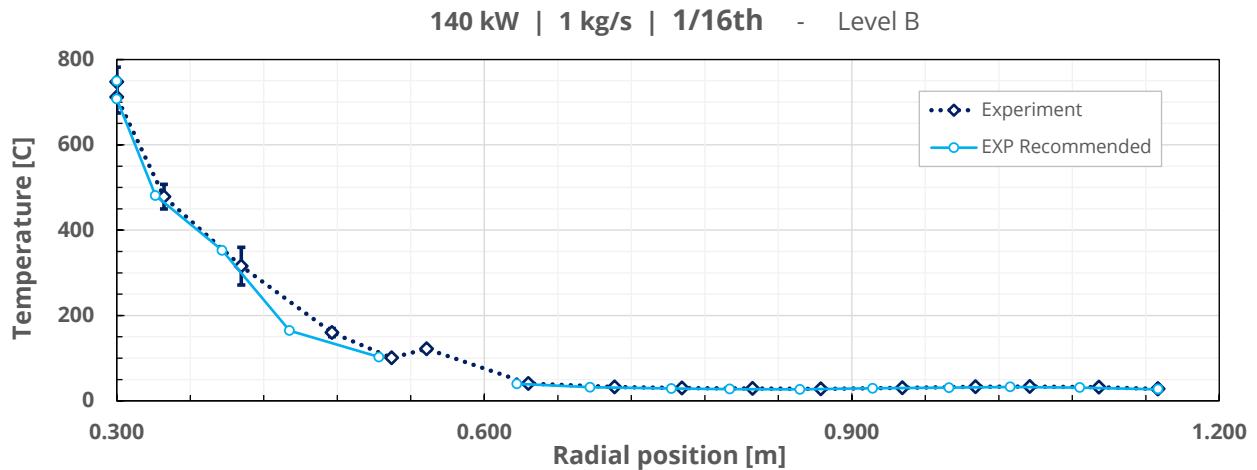


Figure 6.8: Measured temperatures for the 140 kW 1 kg/s forced convection case on Level B.

For each graph on different measurement levels the same convention is taken here. In the next chapter, the same data are used when comparing with the numerical results.

The average and second test measurements for Level C are shown in Figure 6.9.

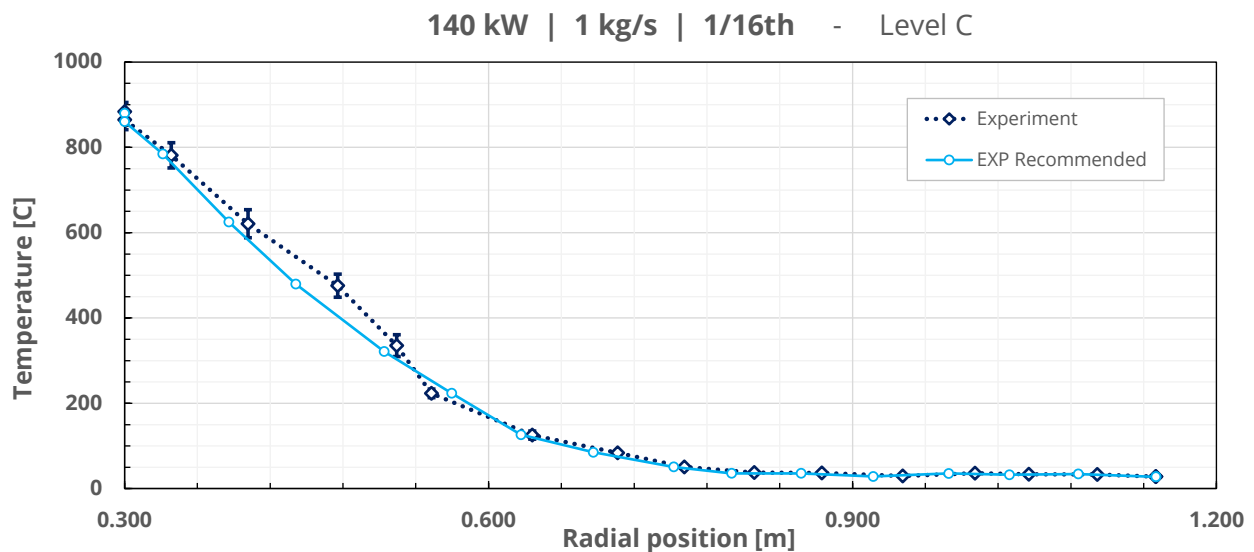


Figure 6.9: Measured temperatures for the 140 kW 1 kg/s forced convection case on Level C.

The average and second test measurements for Level D are shown in Figure 6.10.

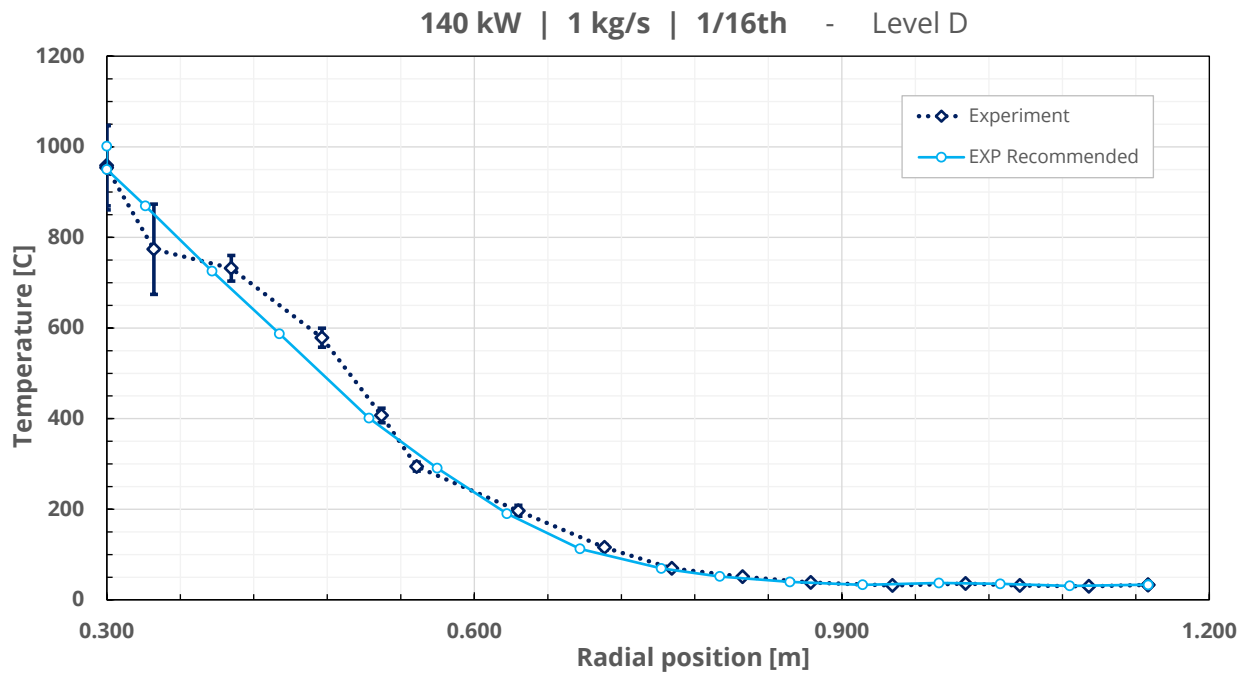


Figure 6.10: Measured temperatures for the 140 kW 1 kg/s forced convection case on Level D.

In the next chapter the numerical results are compared with the experimental measurements as presented here.

End of Chapter

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7. NUMERICAL RESULTS AND COMPARISON

This Chapter presents the numerical results obtained using the two modelling approaches applied to the one isothermal and the three forced convection cases as discussed in Section 4.2.3, together with the corresponding experimental measurements for comparison.

The benchmark case considered is the test case with 140 kW heating and 1 kg/s of coolant flow applied as fraction relative to the 1/16th geometry of the HTTU with discrete flow and heat transfer paths. Experimental measurements from this case were used to calibrate input parameters that have not been determined by relevant equations from literature, in order to achieve the best agreement with the associated experimental values. Furthermore, the results from cases with higher and lower mass flow rates of 2 kg/s and 0.5 kg/s, respectively, are shown in comparison with the corresponding practical measurements, both again at 140 kW of heating. In addition to different mass flows, two cases are presented and compared where the mass flow rate is 1 kg/s but higher heating of 162 kW and lower heating of 120 kW is applied.

7.1. Porous Approach

7.1.1. Isothermal Case with 1 kg/s nitrogen flow

A comparison between measured velocity values for the isothermal 1 kg/s case and numerical results using the porous medium approach, both at 75 mm above the bed, are shown in Figure 7.1 below. It can be seen that in the case of the isothermal flow the flow distribution above packed bed predicted by the porous medium model is in good agreement with the corresponding measured velocity profiles. The notable differences are in the peak velocities near the wall. The porous medium model predicts a smaller peak velocity value near the inner wall and larger peak velocity value near the outer wall. This could be attributed to the fact that the porosities of the inner wall and outer wall regions are outside the upper limit for which the KTA friction factor correlation used in the model, was derived.

In the work of Reger, *et al.* (2024) the numerical results from a high fidelity LES model are used to adapt the KTA correlations for a porous bed focussing on the near-wall region. The work referenced was however not available to disseminate and include in this study for work done in this section at the time. An up-to-date literature overview and inclusion of this referenced work and other recent publications where available shall be looked at in greater detail in a planned follow-up article of the work presented here in the future.

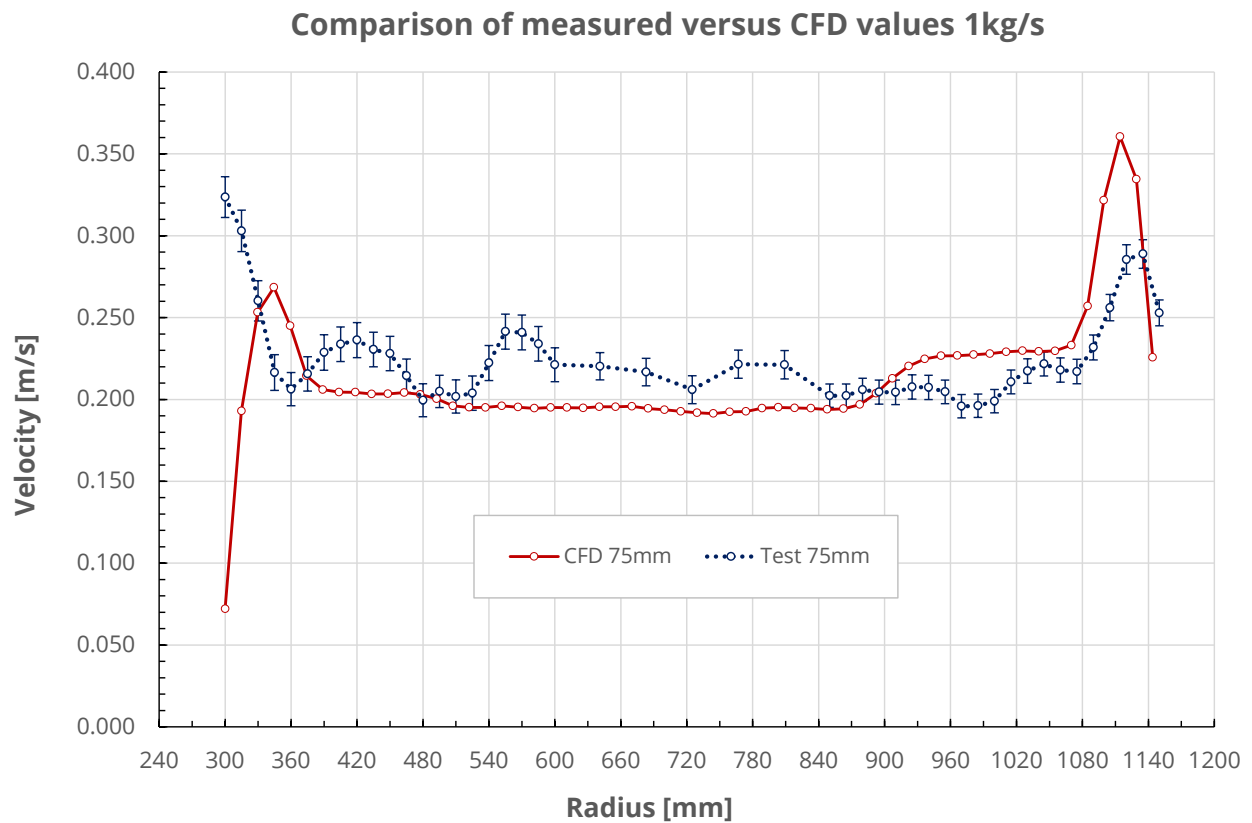


Figure 7.1: Comparison of measured and simulated velocity magnitude for 1 kg/s isothermal at 75 mm.

7.1.2. Forced Convection Case at 140 kW with 1 kg/s nitrogen flow

The numerical temperature results for the forced convection case at 140 kW and nitrogen mass flow rate of 1 kg/s using the porous approach is plotted in Figure 7.2 as “Porous CFD” alongside the corresponding experimental measurements for the 140 kW heating with 1 kg/s forced flow case, at a height equal to that of the “Level D” thermocouples.

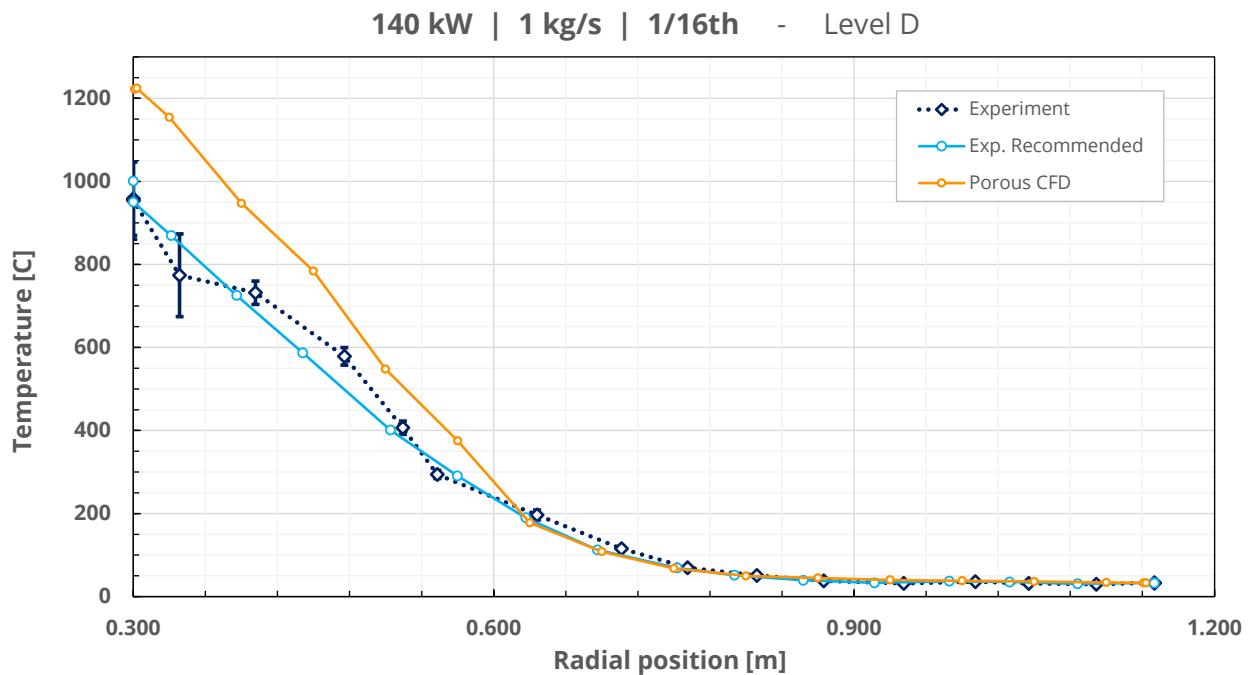


Figure 7.2: Comparison of measured and simulated temperatures for the 140 kW 1kg/s case.

It can be seen in Figure 7.2 that in the bulk and outer wall regions of the packed bed the experimentally measured temperatures and those numerically predicted by the porous approach are in very good agreement. However, in the inner wall and near-wall regions the numerically predicted temperatures are higher than the corresponding measured temperatures. Again, the porosity value being above the limit for the friction factor and Nusselt number correlations could have contributed to this difference. No specific convection and contact heat transfer correlations were implemented at the interface between the wall and the packed bed which further over-predicts temperatures.

As mentioned, other approaches from literature should be considered and investigated in greater detail if this approach is to be applied to the problem at-hand. A porous approach is computationally inexpensive and would allow simulation of larger geometries as is often important in safety studies, such as the inclusion of thermal mass from structures and solid components.

It can be concluded that although the numerically predicted velocities and temperatures using the porous medium approach are in fair to good agreement with the corresponding experimentally measured values, the porous medium model requires further refinement if it is to be relied upon for accurate prediction of temperatures. As the focus of the study is the discrete geometry described in the next section, no further effort was spent on improvement of the porous approach through additional work. A similar approach is taken in the discrete approach of implementing the best-known definitions and parameters at the time of writing.

7.2. Discrete Geometry Approach

7.2.1. Isothermal Case with 1 kg/s nitrogen flow

The numerical results from the discrete geometry simulation for the isothermal case with a nitrogen mass flow rate of 1 kg/s flow is shown in light blue on Figure 7.3 together with the experimentally measured values in dark blue all taken at 75 mm above the bed.

As the measurements are based on averaged values, their standard deviation (indicated with error bars) is relatively low compared to the numerical results which show a large uncertainty due to the large variance of velocity in gaps between spheres in the small section of discrete geometry.

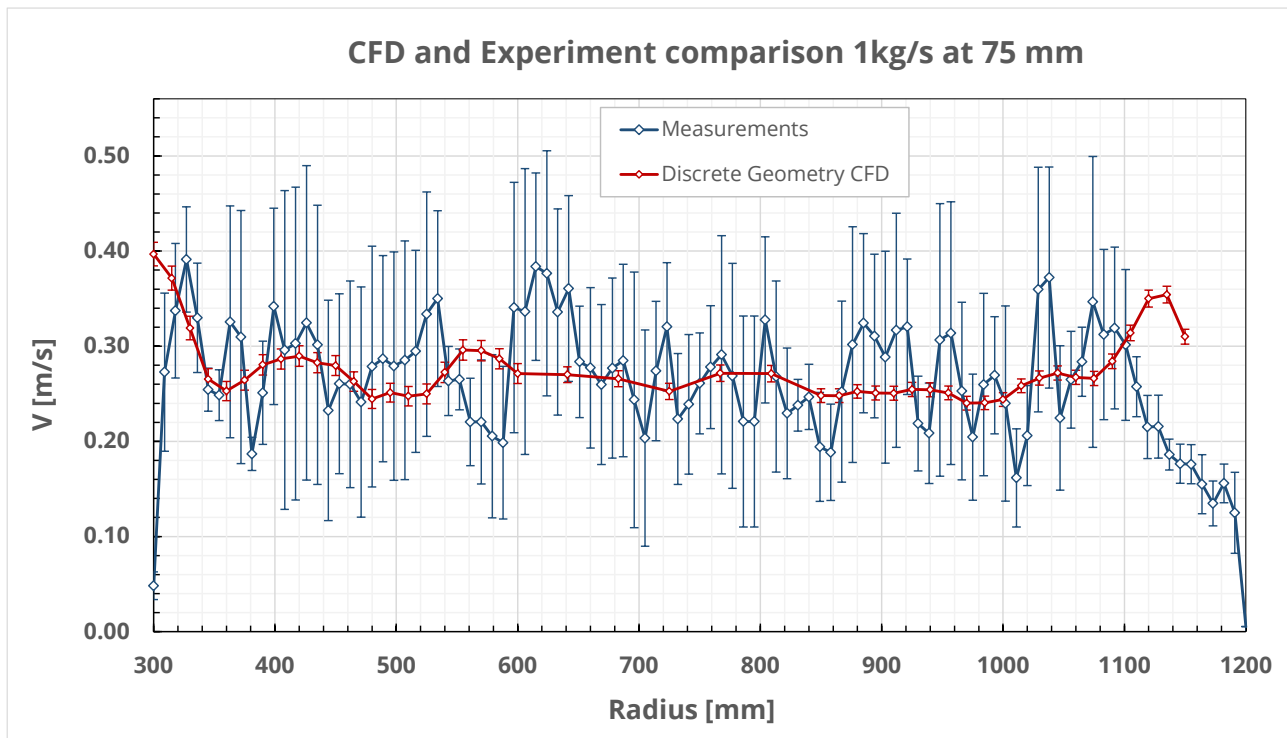


Figure 7.3: Velocity measurements (dark blue) and numerical results of the discrete geometry approach (light blue) at 75mm for the 1 kg/s isothermal case.

Figure 7.3 shows that there is a satisfactory similarity between the experimentally measured velocity profile and corresponding numerically predicted velocity profile, largely within the bounds of uncertainties. The agreement between these values for the velocity peaks in the important vicinity of the inner and outer walls are acceptable. It should be kept in mind that the experimental values are not only the average values for the three radial lines along which the velocities were measured, but each individual measured velocity was a time-averaged measurement taken over a given time period.

It is therefore suggested that a transient numerical simulation should be performed and the time-averaged velocities calculated for each radial position to have a true one-to-one comparison.

7.2.2. Forced Convection Case at 140 kW with 0.5 kg/s nitrogen flow

The numerically predicted temperature distribution for the forced convection case at 140 kW and a nitrogen mass flow rate of 0.5 kg/s is shown in Figure 7.4, where it is compared with the corresponding experimentally measured temperatures.

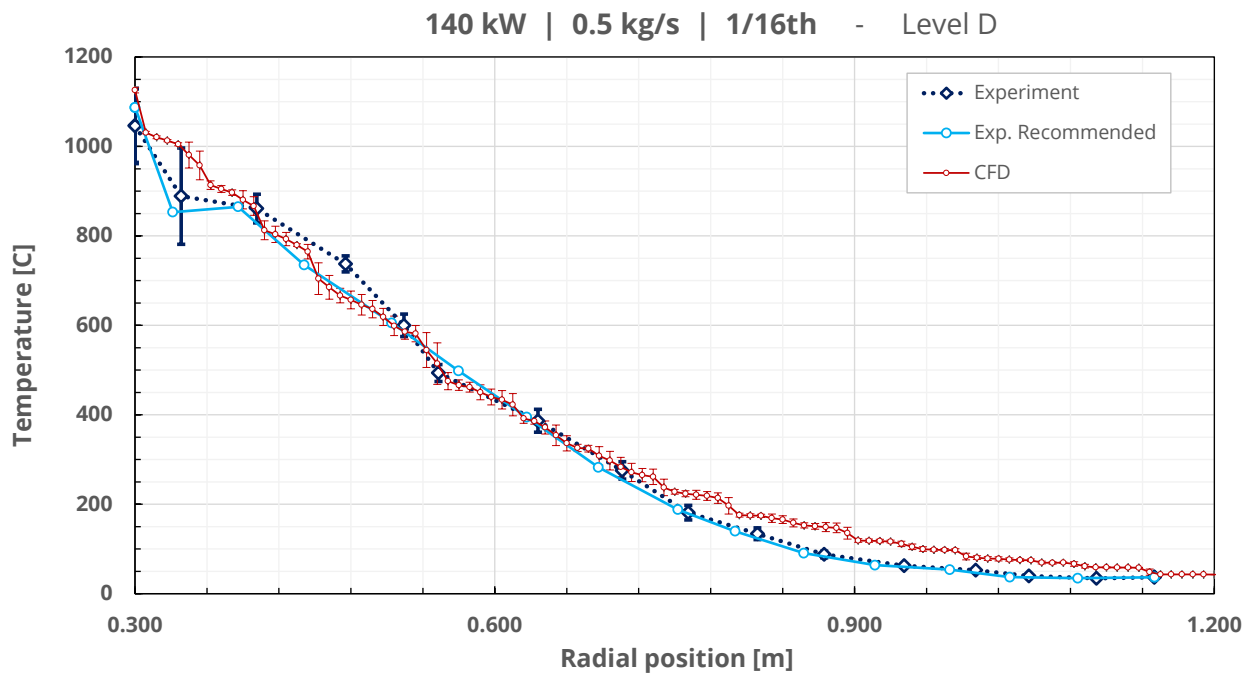


Figure 7.4: Comparison of measured and simulated temperatures for the 140 kW 1kg/s case.

It can be seen in Figure 7.4 in the case of the forced convection simulations of 140 kW heating with coolant flow of 0.5 kg/s that the agreement between the numerically predicted temperatures and the corresponding experimentally measured temperatures is overall very good. There are small deviations – most notably in and around the bulk region. These deviations could in-part be attributed to difference in the porous structure: in the experiments the relevant spheres on a radial line of measurement were aligned, whilst this was not the case in the numerical model with a purely random packing.

7.2.3. Forced Convection Case at 140 kW with 1 kg/s nitrogen flow

The numerically predicted temperature distribution for the forced convection case at 140 kW and 1.0 kg/s nitrogen mass flow rate are shown in Figure 7.5 with comparison to corresponding experimentally measured temperatures.

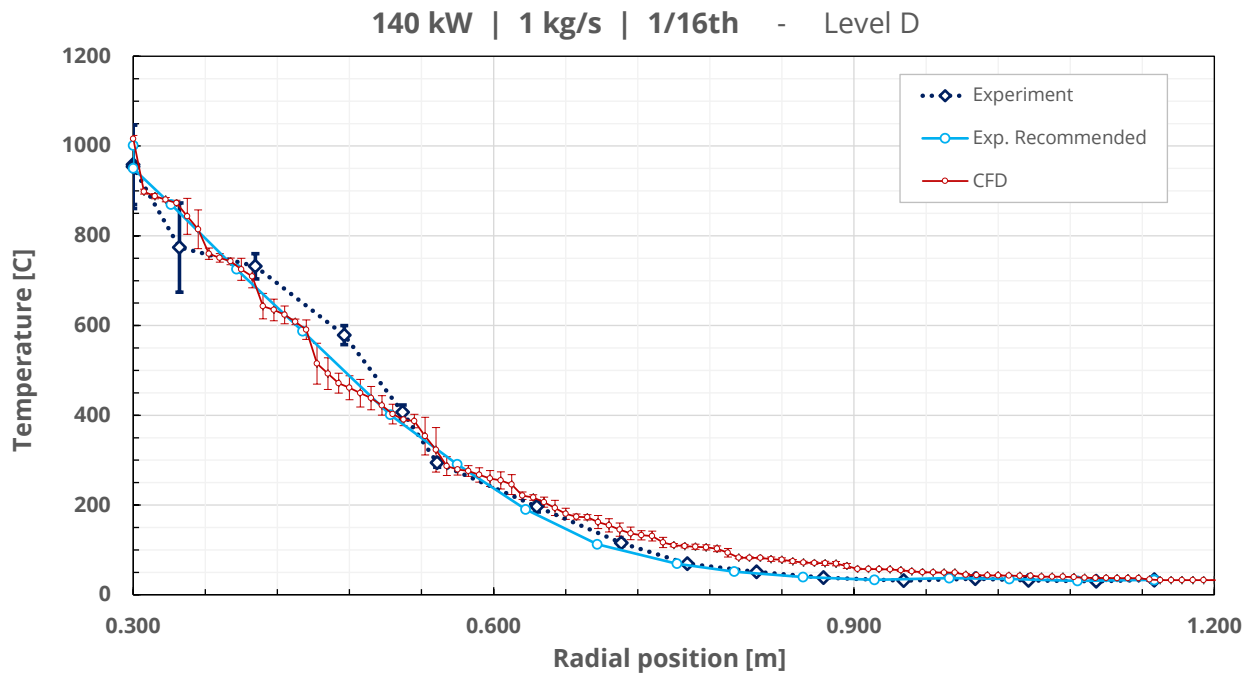


Figure 7.5: Comparison of measured and simulated temperatures for the 140 kW 1kg/s case.

It can be seen in Figure 7.5 that in the case of the forced convection simulation reference case, the agreement between the numerically predicted temperatures and the corresponding experimentally measured temperatures (specifically the “Recommended”) is excellent. Small deviations are again observed in and around the bulk region.

7.2.4. Forced Convection Case at 140 kW with 2 kg/s nitrogen flow

The numerically predicted temperature distribution for the forced convection case at 140 kW and a nitrogen mass flow rate of 2.0 kg/s are shown in Figure 7.6 where it is compared with the corresponding experimentally measured temperatures.

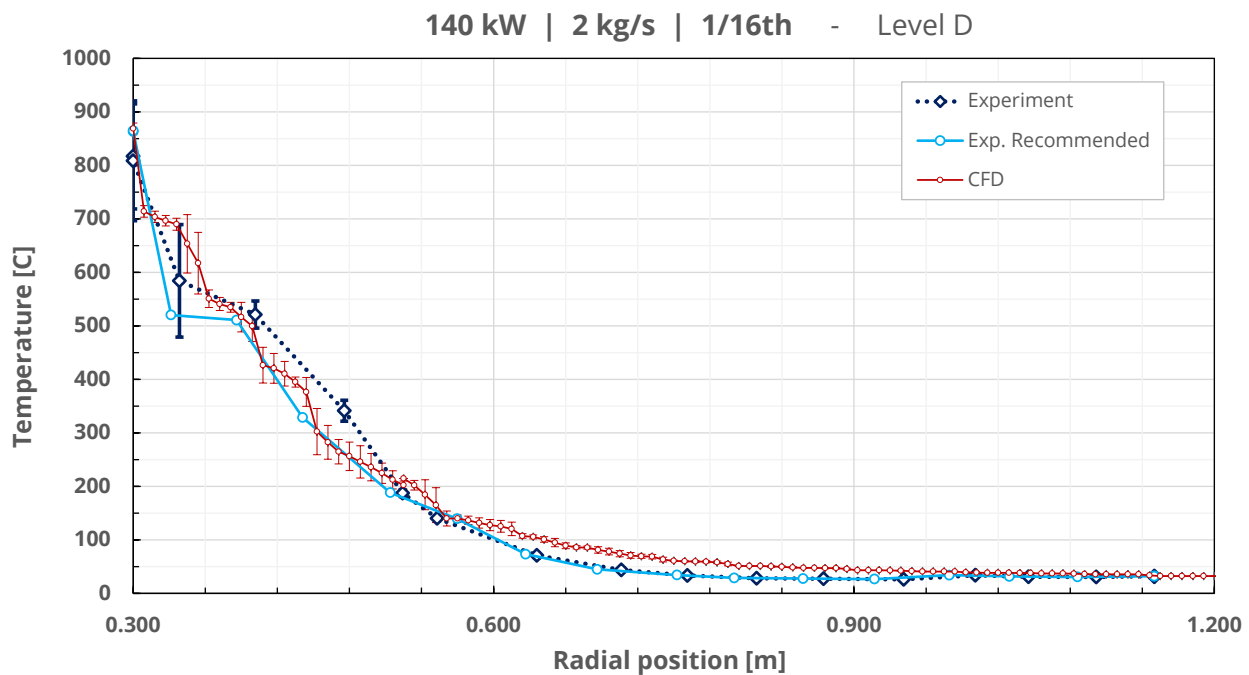


Figure 7.6: Comparison of measured and simulated temperatures for the 140 kW 2kg/s case.

It can be seen in Figure 7.6 in the case of the forced convection simulations, that the agreement between the numerically predicted temperatures and the corresponding experimentally measured temperatures is very good. There are once again small deviations.

Two further cases are presented below at a 16% higher and 17% lower power level, respectively, whilst keeping the mass flow rate the same. For these two cases, full experimental data was not made available and the numerical results are therefore compared to the published measurement points without information on the experimental standard deviation or uncertainties.

7.2.5. Forced Convection Case at 162 kW with 1 kg/s nitrogen flow

The numerically predicted temperature distribution for the forced convection case at 162 kW and nitrogen mass flow rate of 1.0 kg/s are shown in Figure 7.6 where it is compared with the corresponding experimentally measured temperatures. Here there were not sufficient datasets to produce a recommended dataset.

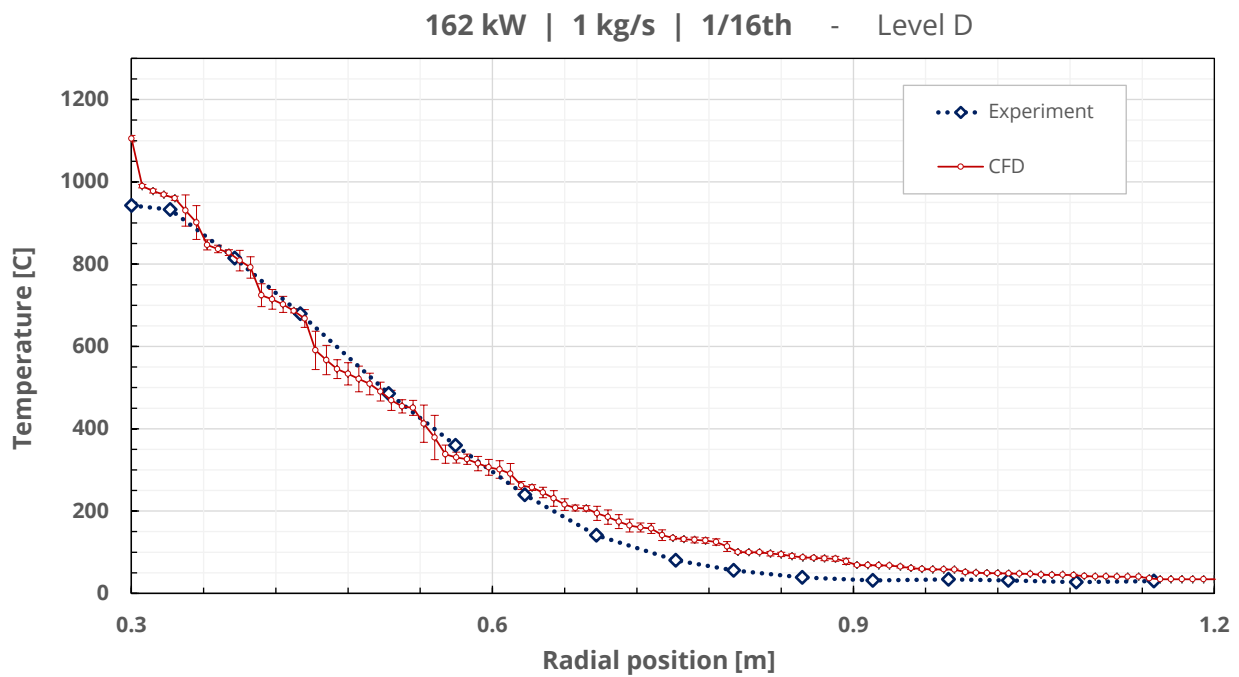


Figure 7.7: Comparison of measured and simulated temperatures for the 162 kW 1kg/s case.

7.2.6. Forced Convection Case at 120 kW with 1 kg/s nitrogen flow

The numerically predicted temperature distribution for the forced convection case at 120 kW and nitrogen mass flow rate of 1.0 kg/s are shown in Figure 7.6 where it is compared with the corresponding experimentally measured temperatures. Due to lack of datasets this case also does not have a recommended set of data.

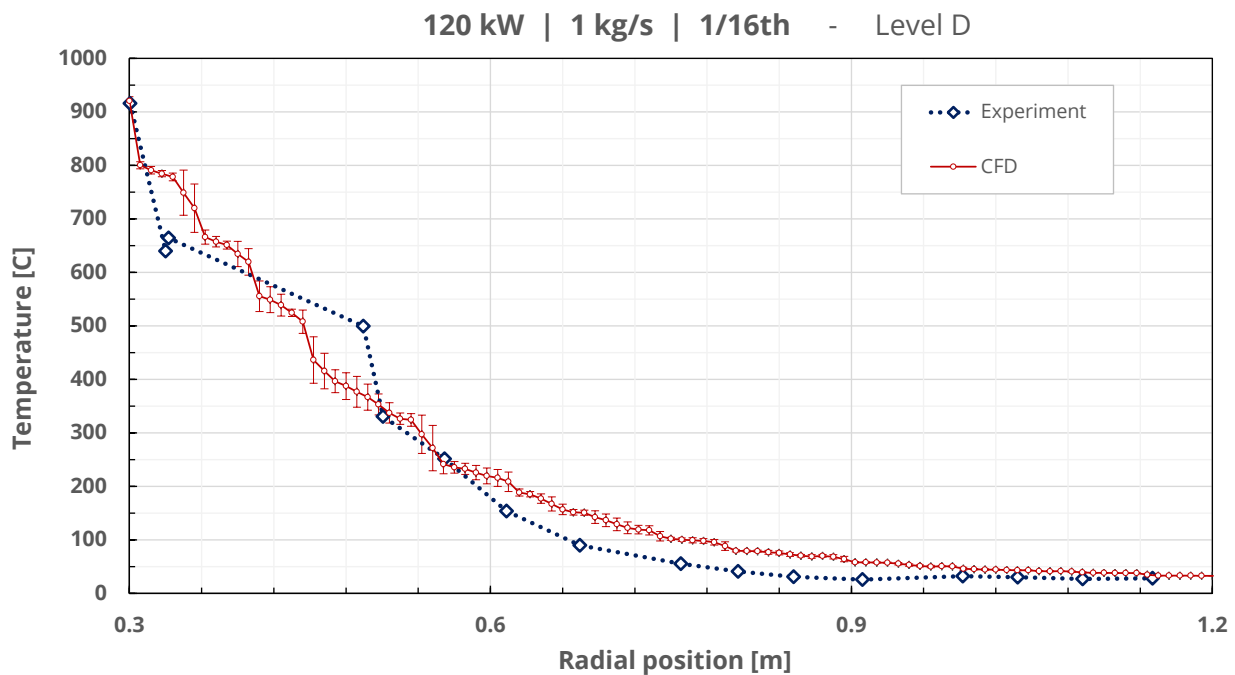


Figure 7.8: Comparison of measured and simulated temperatures for the 120 kW 1kg/s case.

Further good agreement has been shown in these additional cases at higher and lower power levels, thereby demonstrating robustness of the CFD model for cases where the heat flux distribution is varied through the same discrete geometry. The most prevalent differences in all cases can be seen from the near-wall towards the bulk region and within the bulk region itself. These deviations could in part be attributed to difference in the resultant porous structure.

As mentioned, in the experiments the spheres associated with a measurement position were aligned along the radial line in each of the different measurement positions (in level and radial line) so as to be in contact, whilst it was not the case in the numerical model by design as the structure is a result of the random packing.

To quantify the differences, it is suggested that a study be performed where prior to generating the packed bed using DEM, spheres are placed at the positions corresponding to the positions of the instrumented spheres in the experiment. The spheres should be fixed in these positions in order that they do not move when the packed bed is generated. It should then be possible to make more direct comparison between the temperatures of the numerical and experimental spheres in their corresponding positions within the radially varying temperature distribution.

7.3. Verification and Validation

Oberkampf & Trucano (2002) describe the V&V process applied to CFD as the primary means to assess accuracy and validity of simulations. Reasonable efforts have been made in this study following such guidelines as applicable to numerical simulation and experimentation, with much effort and experience already invested in the latter withing the reports consulted.

Verification

A drawback of making use of a commercial software code it that it is not possible to verify the implementation of physics models independently. It is however understood that a large effort is placed on this aspect by developers as it is required for commercial success as well as required by stringent quality assurance requirements.

Beyond the platform provided by the code, all inputs provided by the uses should be thoroughly checked, as was done for this study. Where identified in literature and where the application falls within the range of their defining parameters, correlations have been implemented in the CFD models to account for flow and heat transfer phenomena that cannot be modelled explicitly or need to be supplemented because the geometry does not fully account for them. An example is the stagnant gas in proximity to pebble contact points. In this way the most relevant and recent literature has been applied in an effort to reproduced the measured values from a *best estimate* approach and the numerical models were not 'tuned' to give the results corresponding to the experimental measurements.

As for the discrete geometry cases, the geometry itself has been explicitly defined through DEM and analysed and compared with other means to verify its structure.

Inputs that have been implemented either through in-built tools such as tables or polynomial or with UDF's are mainly:

- Material and fluid properties, including surface emissivity
- Surface roughness, friction and drag coefficients
- Inter-sphere thermal contact resistances, from experimental work by De Beer (2021).

Efforts have been made to verify the correct implementation of the above through the generation of graphs from within the software and compared with the original forms of these and been confirmed to either be completely reproduced in most cases or within less than 1% deviation from the source by comparing point-wise.

Validation

In the benchmark case of 140 kW heating with 1 kg/s forced convection, the simulated temperatures compared very well to that of the measured values in the wall and near-wall regions. Uncertainties in the measurements across different tests equal or exceed those of the numerical values.

The average relative error between numerical and experimental results between 0.3 and 0.6 m radially is 0.9 %, whereas in the range of 0.6 to 1.15 m it is much higher at 38.1 %. Between 0.6 to 0.72 m, this difference falls within the uncertainty range of the numerical values.

Good agreement with experimental measurements within uncertainty makes the model valid and applicable within the range of operational values as demonstrated by the results for the benchmark case. For wider validation, numerical results from the same model were further compared to available experimental data for a wide range of cases where mass flow and power has been varied. These cases were, namely: 0.5 kg/s at 140 kW, 2 kg/s at 140 kW, 1 kg/s at 120 kW, and 1 kg/s at 162 kW.

Further refinements and recommendations deemed valuable through the course of this study as a 'lessons learnt' output, are made in the next chapter.

End of Chapter



8. SUMMARY AND CONCLUSION

In summary of the work presented in the preceding chapters, this chapter discusses the key observations and lists remarks in conclusion of the scope and objectives that were set for this thesis.

8.1. Summary

Very high temperature gas-cooled reactors (VHTGRs) could play a pivotal role in the future of the energy transition away from carbon as several industries relying on high temperature process heat and steam as input. VHTGR plants offer a zero-emission thermal energy source, compared to direct heat from the combustion of coal, oil and gas or indirectly from electricity generated at a lower efficiency from the same sources. Compared to renewables, nuclear has unmatched availability for base load supply and is therefore seen as an important component towards energy sustainability (World Nuclear Association, 2024). Several VHTGR designs have been proposed based on a pebble bed core consisting of spherical fuel elements. Such pebble bed reactors (PBRs) have been built in the past showing promising results. In their design and operation, however, it was noted that there is a large degree of uncertainty around predicted and observed temperatures.

Modern modelling techniques such as computational fluid dynamics (CFD) aim to solve modelling issues of the past, but often come with a large computational expense. Integral effects tests contribute not only to the qualification of next-generation designs but also to the validation of codes including CFD models. The High Temperature Test Unit (HTTU) was an integral effects test of the thermal conduction, radiation and convection in an annular pebble bed, based on the PBMR-400 design.

The scope of this study was limited firstly by the design of the HTTU experiment (Rousseau & Van Staden, 2008) and secondly by the operational envelope of the forced convective tests that were considered. Although natural convection tests were done in the HTTU using helium as well as near-vacuum tests to determine the effective thermal conductivity (Rousseau, *et al.*, 2014), all forced convection tests were only performed with nitrogen. As was shown from the review of literature, there has not been a published study on an annular packed bed experiments under forced convection and therefore previously proposed modelling approaches have not been validated for this type of geometry. The objective of this study was to present two approaches to modelling the integral heat transfer, that is the combined radiative, conduction and convection heat transfer, of the HTTU packed bed under forced convection using Computational Fluid Dynamics and compare the results with the corresponding results of the experiment, taking uncertainty into account as a preliminary validation.

In the literature overview the focus was only the literature of direct relevance to the study. The studies on the porous structure of pebble beds, and the associated thermal-hydraulics and heat transfer in pebble beds were first addressed. Then an overview was given of number of experimental facilities that were constructed and used to perform separate and integral effects tests. The analytical methods and numerical approaches that have been used to model the flow and heat transfer in pebble beds were subsequently discussed.

In Chapter 3 a comprehensive characterization of the variation in the porosity of HTTU annular packed bed was presented. A numerical model of the HTTU annular packed bed consisting of equal sized spheres was generated using the DEM code ESSS Rocky, version 4.3 (ESSS, 2022). The semi-analytical and numerical methods developed by Du Toit (2019b) and Bester & Du Toit (2022) was employed to determine the porosity of the HTTU annular packed bed. An analysis of the radial variation in porosity showed that the results were in good agreement with the experimental results presented by Du Toit (2008) and the results predicted by the correlation of De Klerk (2003). Following the methodology of Bester & Du Toit (2022) the computational domain was divided axially and radially into regions and the average porosity and the standard deviation of the porosity for each region, were calculated. These regional values for the porosity and the standard deviation of the porosity could be implemented in a porous medium CFD model by defining these regions in the set-up of the mesh and assigning the relevant porosity values to the mesh regions.

A porous medium model of the HTTU annular packed bed was constructed accounting for the porosities of the regions into which the packed bed was divided. The CFD code Siemens Simcenter Star-CCM+ (Siemens, 2023) was used to simulate the flow under isothermal conditions and flow heat transfer under non-isothermal conditions. The relevant KTA correlations were employed to account for the flow resistance and convection heat transfer and a correlation derived from HTR-PM experiments to account for the effective thermal conductivity. It was found that the predicted pressure drop over the packed bed was in good agreement with the analytically predicted value. It was also found that in the case of the isothermal flow the flow distribution above packed bed predicted by the porous medium model was good in agreement with the corresponding measured velocity profiles. The notable differences were in the peak velocities near the wall. The porous medium model predicted a smaller peak near the inner wall and larger peak near the outer wall. This could be attributed to the fact that the porosities of the inner wall and outer wall regions are outside the upper limit for which the KTA friction factor correlation was derived. A recommendation for further work is to characterise the sensitivity of the correlation to its different parameter limits, convection is influenced greatly by the local velocity.

In the case of the forced convection simulation, it was found that in bulk and inner wall regions of the packed bed the numerically predicted and experimentally measured temperatures are in very good agreement. However, in the inner wall region the numerically predicted temperatures are higher than the corresponding measured temperatures. Again, the porosity value being above the limit for the friction factor and Nusselt number correlations could have contributed to the difference. No specific convection and contact heat transfer correlations were implemented at the interface between the wall and the packed bed. This will have to be investigated in detail.

An explicit model of the HTTU annular packed bed was also constructed where the packing of the spheres was generated using a DEM code and the flow and spheres thus modelled explicitly in detail. The CFD code Siemens Simcenter Star-CCM+ (Siemens, 2023) was again used to simulate the flow under isothermal conditions and flow heat transfer under non-isothermal conditions. The only correlation implemented accounted for the contact resistance between adjacent spheres and between the walls and spheres in contact with the walls. It was again found that the predicted pressure drop over the packed bed was in good agreement with the analytically predicted value. In the case of the isothermal flow, it was found that there was a satisfactory similarity between the experimentally measured velocity profile and corresponding numerically predicted velocity profile. The agreement between the values for the velocity peaks near the inner and outer walls are good. It should be kept in mind that the experimental values are not only the average values for the three radial lines along which the velocities were measured, but each individual measured velocity was a time-averaged measurement taken over a given time period. It is therefore suggested that a transient numerical simulation should be performed and the time-averaged velocities calculated for each radial position. In the case of the forced convection simulation, it was found that agreement between the numerically predicted temperatures and the corresponding experimentally measured temperatures is very good. There are small deviations. These deviations could in part be attributed to difference in the porous structure. In the experiments the relevant spheres of a radial line were aligned, whilst it was not the case in the numerical model.

Statement on the unique contribution of this work in the field

The unique contribution of this study is highlighted as it being the first time that the HTTU experiment's integral heat transfer is modelled with CFD and thereby lending further insights into heat transport in annular packed beds and the validity of the various inputs and assumptions – bringing the different aspects that have been studied separately, together.

8.2. Recommendations for further work

Initially the intent of this study was to model the full HTTU, including its vessel and internals, using only a porous medium approach. This choice was due to computational resource limitations which would have made a model of the entire bed and surrounding structures, using a discrete geometry approach, intractable. It was found that the results from using the porous approach were not in good agreement with measurements using standard (yet outdated by modern standards) correlations and an approximated porosity distribution.

For this reason, first a $1/8^{\text{th}}$ and finally a $1/16^{\text{th}}$ geometry with discrete solid and gas phases was developed and which could be simulated on the available computational resources. The obtained results were promising in both cases but it was evident that with integral heat transfer models implemented to concurrently solve for convection, radiation and conduction that execution of the $1/8^{\text{th}}$ model would be too resource-intensive and so efforts were focussed on the smaller $1/16^{\text{th}}$ section as presented in previous chapters.

It is therefore recommended that, in the case of the porous medium approach, a comprehensive study be conducted to find suitable correlations for the pressure drop and convection heat transfer that could account for larger and varied porosities. The heat transfer between the wall and bed regions must also be investigated in more detail, as has been done in more recent literature than was available at the time of conducting the work described in Section 7.1.1.

As mentioned in Section 7.2.1, the experimental velocity measurements in the isothermal case were time-averaged whereas the compared numerical values were steady-state. It was observed that the local absolute velocities were varying however, due to vortex shedding of the turbulent flow through the top-most level of spheres. The suggestion was therefore made that the numerical simulation also be done as transient and the time-averaged velocities as well as the standard deviation for a certain time be used to compare against the experimental measurements for a true comparison. Although the results were acceptable to be used to continue into the forced convection part of the study, this is a recommended point of improvement to have a quantitative comparison for the isothermal case in terms of velocities.

In the case of the explicit / discrete geometry approach it is recommended that, prior to generating the packed bed using DEM, spheres are placed at the positions corresponding with the positions of the instrumented spheres in the experiment. The spheres should be fixed in these positions in order to not move when the rest of the packed bed is generated. It should then be possible to make a more direct comparison between the temperatures of the aligned numerical and aligned experimentally measured spheres. This is to firstly address the question about worse agreement between numerical and measured values in the bulk region, compared to those in the near-wall high-temperature zone.

The focus of this study was to be limited to workstation-level hardware and feasibility of corresponding model fidelity, which has been demonstrated. Where a larger geometry is concerned, it is certainly possible to follow the same methodology to simulate a full pebble bed core, but would inevitably require high performance computing hardware. A formal uncertainty quantification of the several parameters related to the mesh and numerical model definition would be advisable and to evaluate the performance of higher fidelity models, first with a comparable geometry before increasing scope.

Considering other experimental campaigns conducted using the HTTU experiment, tests were also conducted at near-vacuum (to determine the effective thermal conductivity) but also in natural convection in different tests where nitrogen and also helium were used. Modelling of the vacuum and the natural convection cases using discrete geometry CFD could give insights into the phenomena involved through a fundamental comparison of results with the absence of certain separate effects.

Lastly, several other codes exist that make use of a porous medium approach to model packed beds. It is the intention of the author to further compare the results from these methods, applied to the HTTU in forced convection, to those presented in this study in further work.

8.3. Concluding Remarks

Feasibility

The feasibility of using a “moderate” (in terms of computational expense) RANS approach with medium mesh size to achieve acceptable results on workstation-grade hardware was demonstrated. This presents to the option of using modern simulation tools with acceptable accuracy to contribute to the qualification and safety analyses of the next generation of Pebble Bed Reactors.

Reliance on Analytical Methods

The KTA standards as an analytical method have been validated and widely accepted yet a high uncertainty in certain areas such as the near-wall and porous pockets remain. Further work is needed to convince regulatory bodies on the applicability and validity of numerical methods.

It is also hoped that the HTTU experiments could become a reference case similar to that of the SANA experiment from Stöcker & Nießen (1997).

R&D on Numerical Methods

This work is closed out with a quote from the chapter on Pebble Bed Gas Cooled Reactors in the *Encyclopedia of Nuclear Energy*, Volume 1 by F. Reitsma (2021). The section discusses the major challenges and the need for R&D in the field – highlighting the successful role that software and simulation has played in this regard:

"Finally, R&D on improved software codes and simulation methods are continuing to reduce uncertainties and improve the verification and validation status of these codes through benchmarking and comparisons with experiments and plant data."

End of Chapter



LIST OF REFERENCES

- Abdulmohsin, R. S. & Al-Dahhan, M. H., 2015. Characteristics of convective heat transport in a packed pebble-bed reactor. *Nuclear Engineering and Design*, Volume 284, pp. 143-152.
- Abdulmohsin, R. S. & Al-Dahhan, M. H., 2016. Axial dispersion and mixing phenomena of the gas phase in a packed pebble-bed reactor. *Annals of Nuclear Energy*, Volume 88, pp. 100-111.
- Abdulmohsin, R. S. & Al-Dahhan, M. H., 2016. Corrigendum to "Characteristics of convective heat transport in a packed pebble-bed reactor" [Nucl. Eng. Des. 284 (2015) 143–152]. *Nuclear Engineering and Design*, Volume 305, p. 723.
- Achenbach, E., 1995. Heat and Flow Characteristics of Packed Beds. *Experimental and Thermal and Fluid Science*, Volume 10, pp. 17-27.
- Ahmadi Motlagh, A. H. & Hashemabadi, S. H., 2008. 3D CFD simulation and experimental validation of particle-to-fluid heat transfer in a randomly packed bed of cylindrical particles. *International Communications in Heat and Mass Transfer*, Volume 35, pp. 1183-1189.
- Al Falahi, F. & Al-Dahhan, M., 2016. Experimental investigation of the pebble bed structure by using gamma ray tomography. *Nucl. Eng. Des.*, Volume 310, pp. 231-246.
- Allelein, H.-J. & Verfondern, K., 2018. Major milestones of HTR development in Germany and still open research issue. *Annals of Nuclear Energy*, Volume 116, pp. 114-127.
- Almusafir, R. S., Jasim, A. A. & Al-Dahhan, M. H., 2023. Review of the Fluid Dynamics and Heat Transport Phenomena in Packed Pebble Bed Nuclear Reactors. *Nuclear Science and Engineering*, 197(6), pp. 1001-1037.
- Amini, N. & Hassan, Y. A., 2014. Experimental study of bypass flow in near wall gaps of a pebble bed reactor using hot wire anemometry technique. *Annals of Nuclear Energy*, Volume 65, pp. 60-71.
- Ansys, Inc., 2024a. *Ansys Fluent Fluid Simulation Software*. [Online] Available at: <https://www.ansys.com/products/fluids/ansys-fluent> [Accessed 11 November 2024].
- Ansys, Inc., 2024b. *Ansys CFX Turbomachinery CFD Software*. [Online] Available at: <https://www.ansys.com/products/fluids/ansys-cfx> [Accessed 11 November 2024].
- Auwerda, G. J., 2014. *Core Physics of Pebble Bed High Temperature Nuclear Reactors*, Delft, The Netherlands: Delft University of Technology.
- Auwerda, G. J., Kloosterman, J.-L., Lathouwers, D. & Van Der Hagen, T. H. J. J., 2013. Macroscopic and microscopic packing properties of experimental and computational pebble beds. *Nuclear Technology*, 183(3), pp. 272-286.
- Auwerda, G. J., Kloosterman, J. L., Lathouwers, D. & Van der Hagen, T. H. J. J., 2010a. Effects of random pebble distribution on the multiplication factor in HTR pebble bed reactors. *Annals of Nuclear Energy*, 37(8), pp. 1056-1066.

- Auwerda, G. J. et al., 2010b. *Comparison of Experiments and Calculations of Void Fraction Distributions in Randomly Stacked Pebble Beds*. Pittsburgh, PA, United States of America, Int. Conf. on the Physics of Reactors 2010 (PHYSOR 2010), pp. 1897-1909.
- Bahrami, M., Yovanovich, M. M. & Culham, J. R., 2005. A Compact Model for Spherical Rough Contacts. *Journal of Tribology*, 127(4), pp. 844-889.
- Bahrami, M., Yovanovich, M. M. & Culham, J. R., 2006. Effective thermal conductivity of rough spherical packed beds. *International Journal of Heat and Mass Transfer*, 49(19-20), pp. 3691-3701.
- Balakrishnan, A. R. & Pei, D. C. T., 1978. Heat Transfer in Gas-Solid Packed Bed Systems - 1. A Critical Review. *Ind. Eng. Chem. Process Des. Dev.*, 18(1), pp. 30-40.
- Barker, J. J., 1965. Heat Transfer in Packed Beds. *Industrial & Engineering Chemistry*, 57(4), pp. 43-51.
- Bauer, R. & Schlünder, E. -U., 1978. Effective radial thermal conductivity of packings in gas flow, Part II: thermal conductivity of the packing fraction without gas flow. *Int. Chem. Engng.*
- Becker, S. & Laurien, E., 2003. Three-dimensional numerical simulation of flow and heat transport in high-temperature nuclear reactors. *Nuclear Engineering and Design*, Volume 222, pp. 189-201.
- Benenati, R. F. & Brosilow, C. B., 1962. Void Fraction Distribution in Beds of Spheres. *A.I.Ch.E. J.*, 8(3), pp. 359-361.
- Bester, P. M., 2022. *Analysis of the radial, axial and tangential porosity variations of packed beds of spheres*, Potchefstroom: North-West University.
- Bester, P. M. & Du Toit, C. G., 2022. A methodology to analyse the angular, radial and regional porosities of a cylindrical packed bed of spheres. *Nucl. Eng. Des.*, Volume 392, p. 111766.
- Bester, P. M., Du Toit, C. G. & Potgieter, M. C., 2021. A numerical analysis of the porosity of the HTR-10 packed pebble bed. *Nucl. Eng. Des.*, Volume 383, p. 111438.
- Bey, O. & Eigenberger, G., 1997. Fluid flow through catalyst filled tubes. *Chemical Engineering Science*, 52(8), pp. 1365-1376.
- Brähler, G. et al., 2012. Improvements in the fabrication of HTR fuel elements. *Nuclear Engineering and Design*, Volume 251, pp. 239-243.
- Breitbach, G. & Barthels, H., 1980. Radiant heat transfer in the high temperature reactor core after failure of the afterheat removal systems. *Nuclear Technology*, 49(3), pp. 392-399.
- Bu, S. S. et al., 2014. On contact point modifications for forced convective heat transfer analysis in a structured packed bed of spheres. *Nuclear Engineering and Design*, Volume 270, pp. 21-33.
- Carman, P. C., 1937. Fluid flow through granular beds. *Transactions of the Institution of Chemical Engineers*, Volume 15, pp. 150-166.
- Carman, P. C., 1997. Fluid flow through granular beds. *Chemical Engineering Research and Design*, 75(Supplement), pp. S32-S48.
- Chen, F. & Han, Z., 2021. Steady-state thermal fluids analysis for the HTR-PM equilibrium core. *International Journal of Advanced Nuclear Reactor Design and Technology*, Volume 3, pp. 11-17.
- Chen, L. & Lee, J., 2017. Experimental analysis of the thermal field and heat transfer characteristics of a pebble-bed core in a high-temperature gas-cooled reactor. *Annals of Nuclear Energy*, Volume 110, pp. 338-348.

- Cohen, Y. & Metzner, A. B., 1981. Wall effects in Laminar flow of fluids through packed beds. *A.I.Ch.E. J.*, 27(5), pp. 705-715.
- Coutelieris, F. A. & Delgado, J. M. P. Q., 2012. *Transport Processes in Porous Media*. Berlin, Germany: Springer.
- Dahl, P. M. & Su, J., 2017. *Simulation in CFD of a Pebble Bed - Advanced High Temperature Reactor Core using OpenFOAM*. Belo Horizonte, Brazil, INAC.
- Daniels, F., 1957. *Neutronic Reactor System*. United States of America, Patent No. 2809931.
- Daszkowski, T. & Eigenberger, G., 1992. A reevaluation of fluid flow, heat transfer and chemical reaction in catalyst filled tubes. *Chemical Engineering Science*, Volume 47, pp. 2245-2250.
- De Beer, M., 2021. *Characterisation of the effective thermal conductivity in the near wall region of a packed pebble bed*, Potchefstroom: North-West University.
- De Beer, M., Du Toit, C. G. & Rousseau, P. G., 2017. A methodology to investigate the contribution of conduction and radiation heat transfer to the effective thermal conductivity of packed graphite pebble beds, including the wall effect. *Nuclear Engineering and Design*, Volume 314, pp. 67-81.
- De Beer, M., Du Toit, C. G. & Rousseau, P. G., 2018. Experimental study of the effective thermal conductivity in the near-wall region of a packed pebble bed. *Nuclear Engineering and Design*, Volume 339, pp. 253-268.
- De Klerk, A., 2003. Voidage Variation in Packed Beds at Small Column to Particle Diameter Ratio. *A.I.Ch.E. J.*, 49(8), pp. 2022-2029.
- Dixon, A. G., Nijemeisland, M. & Stitt, E. H., 2013. Systematic mesh development for 3D CFD simulation of fixed beds: Contact points study. *Computers and Chemical Engineering*, Volume 48, pp. 135-153.
- Dong, Z. et al., 2018. Dynamical modeling and simulation of the six-modular high temperature gas-cooled reactor plant HTR-PM600. *Energy*, Volume 155, pp. 971-991.
- Du Toit, C. G., 2002. *Numerical Determination of the Variation in the Porosity of the Pebble-Bed Core*. Petten, The Netherlands, Proceedings of the 1st International Topical Meeting on High Temperature Reactor Technology (HTR 2002), pp. 287-291.
- Du Toit, C. G., 2008. Radial variation in porosity in annular packed beds. *Nucl. Eng. Des.*, Volume 238, pp. 3073-3079.
- Du Toit, C. G., 2019a. *Analysing the porosity of a pebble bed core using a combined analytical and numerical approach*. Juan-les-pins, France, Proceedings of the 2019 International Congress on Advances in Nuclear Power Plants (ICAPP 2019).
- Du Toit, C. G., 2019b. Analysing the porous structure of packed beds of spheres using a semi-analytical approach. *Powder Technol.*, Volume 342, pp. 475-485.
- Du Toit, C. G. & Rousseau, P. G., 2014. *Separate Effects Tests to Determine the Pressure Drop over Packed Beds in the PBMR HPTU Test Facility*. Weihai, China, Proceedings of the HTR 2014.
- Du Toit, C. G., Rousseau, P. G., Greyvenstein, G. P. & Landman, W. A., 2006. A systems CFD model of a packed bed high temperature gas-cooled nuclear reactor. *International Journal of Thermal Sciences*, Volume 45, pp. 70-85.

- Du Toit, C. G., Rousseau, P. G. & Kgame, T. L., 2014. Separate effects tests to determine the thermal dispersion in structured pebble beds in the PBMR HPTU test facility. *Nuclear Engineering and Design*, Volume 271, pp. 437-443.
- Du Toit, C. G., Van Loggerenberg, P. J. & Vermaak, H. J., 2021. An evaluation of selected friction factor correlations and results for the pressure drop through random and structured packed beds of uniform spheres. *Nuclear Engineering and Design*, Volume 379, p. 111213.
- Duchnowski, E. M. & Brown, N. R., 2024. A review of multiphysics tools and methods to evaluate high temperature pebble bed reactors. *Progress in Nuclear Energy*, Volume 171, p. 105164.
- Eisfeld, B. & Schnitzlein, K., 2001. The influence of confining walls on the pressure drop in packed beds. *Chemical Engineering Science*, 56(14), pp. 4321-4329.
- Elder, R. & Allen, R., 2009. Nuclear heat for hydrogen production: Coupling a very high/high temperature reactor to a hydrogen production plant. *Progress in Nuclear Energy*, 51(3), pp. 500-525.
- Erdim, E., Akgiray, Ö. & Demir, İ., 2015. A revisit of pressure drop-flow rate correlations for packed beds of spheres. *Powder Technology*, Volume 283, pp. 488-504.
- Ergun, S., 1952. Fluid Flow Through Packed Columns. *Chemical Engineering Progress*, 48(2), pp. 89-94.
- Ergun, S. & Orning, A. A., 1949. Fluid Flow through Randomly Packed Columns and Fluidized Beds. *Industrial and Engineering Chemistry*, 41(6), pp. 1179-1184.
- ESSS, 2022. *Rocky Release 2022 R2, DEM Technical Manual*. Florianópolis, Brazil: ESSS Rocky DEM, S.R.L..
- Fahien, R. W., 1983. *Fundamentals of Transport Phenomena*. 1st ed. s.l.:McGraw-Hill.
- Feng, Y. et al., 2021. Effects of bed dimension, friction coefficient and pebble size distribution on the packing structures of the pebble bed for solid tritium breeder blanket. *Fusion Eng. Des.*, Volume 163, p. 112156.
- Filippov, G. A., Bogoyavlenskii, R. G., Ponomarev-Stepnoi, N. N. & Gol'tsev, A. O., 2004. Modular High-Temperature Helium-Cooled Nuclear Reactor with Spherical Fuel Elements for Electricity and Hydrogen Production. *Atomic Energy*, Volume 96, p. 152-158.
- Fischer, P. et al., 2022. NekRS, a GPU-accelerated spectral element Navier-Stokes solver. *Parallel Computing*, Volume 114, p. 102982.
- Gao, Z. & Shi, L., 2002. Thermal hydraulic transient analysis of the HTR-10. *Nuclear Engineering and Design*, 218(1-3), pp. 65-80.
- Generation IV International Forum, 2024. *Generation IV Goals, Technologies and GIF R&D Roadmap: Very High Temperature Reactor (VHTR)*. [Online]
Available at: <https://www.gen-4.org/generation-iv-criteria-and-technologies/very-high-temperature-reactor-vhtr>
[Accessed 7 November 2024].
- Giese, M., Rottschäfer, K. & Vortmeyer, D., 1998. Measured and Modeled Superficial Flow Profiles in Packed Beds with Liquid Flow. *A.I.Ch.E. J.*, 44(2), pp. 484-490.
- Gnielinski, V., 1981. Equations for the calculation of heat and mass transfer during flow through stationary spherical packings at moderate and high Peclet numbers. *Int Chem Eng*, 21(3), pp. 378-383.

- Gnielinski, V., 2010. G9 Fluid-Particle Heat Transfer in Flow Through Packed Beds of Solids (in: VDI Heat Atlas Part G - Forced Convection). In: V. V. u. Chemieingenieurwesen, ed. *VDI Heat Atlas, 2nd Edition*. Berlin; Heidelberg: Springer-Verlag, pp. 743-744.
- Golovko, V. F., Kiryushin, A. I., Kodochigov, N. G. & Kuzavkov, N. G., 1996. *State of HTGR development in Russia*. Nizhny Novgorod, Russian Federation, OKB Mechanical Engineering.
- Goodling, J. S. et al., 1983. Radial Porosity Distribution in Cylindrical Beds Packed with Spheres. *Powder Technol.*, 35(1), pp. 23-29.
- Govindarao, V. M., Subbanna, M., Rao, A. V. & Ramrao, K. V., 1990. Voidage profile in packed beds by multi-channel model: effects of curvature of the channels. *Chem. Eng. Sci.*, 45(1), pp. 362-364.
- Greyvenstein, G. P., Rousseau, P. G. & Nicholls, D., 2003. Design and successful testing of a physical model of the Pebble Bed Modular Reactor. *International Journal for Nuclear Power*, Volume 2, pp. 105-110.
- Gunn, D. J., 1987. Axial and radial dispersion in fixed beds. *Chemical Engineering Science*, 42(2), pp. 363-373.
- Guo, Z. et al., 2017. Radial porosity peak at the centerline of packed beds with small tube to particle diameter ratios. *Powder Technol.*, Volume 319, pp. 445-451.
- Hao, C., Yang, R. & Cheng, Y., 2022. Uncertainty analysis of keff due to the random packing of pebbles in the pebble bed HTR. *Nuclear Engineering and Design*, Volume 398, p. 111992.
- Hassan, Y. A., 2008. Large eddy simulation in pebble bed gas cooled core reactors. *Nuclear Engineering and Design*, Volume 238, pp. 530-537.
- Hassan, Y. A. & Dominguez-Ontiveros, E. E., 2008. Flow visualization in a pebble bed reactor experiment using PIV and refractive index matching techniques. *Nuclear Engineering and Design*, 238(11), pp. 3080-3085.
- Hoffmann, J. E. & Janse van Rensburg, J. J., 2006. *Verification and Validation of the CFD model of the PBMR reactor*. Johannesburg, South Africa, 3rd International Topical Meeting on High Temperature Reactor Technology.
- Howell, J. R., Mengüç, M. P., Daun, K. & Siegel, R., 2021. *(On-line Appendices to) Thermal Radiation Heat Transfer*. 7th Edition ed. s.l.:Taylor and Francis.
- Hunt, M. L. & Tien, C. L., 1990. Non-Darcian Flow, Heat and Mass Transfer in Catalytic Packed-Bed Reactor. *Chem. Eng. Sci.*, 45(1), pp. 55-63.
- IAEA, 2003. *Evaluation of high temperature gas cooled reactor performance: Benchmark analysis related to initial testing of the HTTR and HTR-10*, Vienna, Austria: International Atomic Energy Agency.
- IAEA, 2013. *TECDOC-1694 Evaluation of High Temperature Gas Cooled Reactor Performance: Benchmark Analysis Related to the PBMR-400, PBMM, GT-MHR, HTR-10 and the ASTRA Critical Facility*, Vienna, Austria: International Atomic Energy Agency.
- IAEA, 2024. *Power Reactor Information System - China - Shidao Bay-1*. [Online]
Available at: <https://pris.iaea.org/pris/CountryStatistics/ReactorDetails.aspx?current=957>
[Accessed 11 November 2024].
- Idaho National Engineering Laboratory, 1995. *RELAP5/MOD3 Code Manual Volume 1*, Idaho Falls, ID: Lockheed Idaho Technologies Company.
- Idaho National Laboratory, 2010. *NGNP Fuel Qualification White Paper*, s.l.: U.S. Department of Energy.

- Jafari, A., Zamankhan, P., Mousavi, S. M. & Pietarinen, K., 2008. Modeling and CFD simulation of flow behavior and dispersivity through randomly packed bed reactors. *Chemical Engineering Journal*, 144(3), pp. 476-482.
- Janse van Rensburg, J. J. & Kleingeld, M., 2011. An integral CFD approach for the thermal simulation of the PBMR Reactor Unit. *Nuclear Engineering and Design*, 241(8), pp. 3130-3141.
- Jerier, J.-F., Richefeu, V., Imbault, D. & Donzé, F.-V., 2010. Packing spherical discrete elements for large scale simulations. *Comput. Methods Appl. Mech. Eng.*, 199(25-28), pp. 1668-1676.
- Jun, J. S., Lim, H. S. & Lee, W. J., 2007. *The GAMMA Code Assessment of the HTR-10 Safety Demonstration Experiments – LOFC ATWS*. PyeongChang, Korea, Transactions of the Korean Nuclear Society Autumn Meeting.
- Jun, J. S., Lim, H. S. & Lee, W. J., 2009. The benchmark calculations of the gamma+ code with the HTR-10 safety demonstration experiments. *Nuclear Engineering and Technology*, 41(3), pp. 307-318.
- Jurtz, N., Kraume, M. & Wehinger, G. D., 2019. Advances in fixed-bed reactor modeling using particle-resolved computational fluid dynamics (CFD). *Reviews in Chemical Engineering*, 35(2), pp. 139-190.
- Kadak, A. C., 2007. MIT Pebble Bed Reactor Project. *Nuclear Engineering and Technology*, 39(2), pp. 95-102.
- Kleiber, M. & Joh, R., 2010. D3: Properties of Pure Fluid Substances, D3.1 Liquids and Gases (in: VDI Heat Atlas Part D - Thermophysical Properties). In: V. V. u. Chemieingenieurwesen, ed. *VDI Heat Atlas, 2nd Edition*. Berlin; Heidelberg: Springer-Verlag, pp. 301-385.
- Kolev, N., 2006. *Packed Bed Columns; For Absorption, Desorption, Rectification and Direct Heat Transfer*. 1 ed. Sofia, Bulgaria: Elsevier Science.
- Kreyszig, E., 2006. *Advanced Engineering Mathematics*. 9th International Edition ed. Hoboken, NJ, United States of America: John Wiley & Sons.
- KTA, 1978. *Reactor Core Design for High-Temperature Gas-Cooled Reactors Part 1: Calculation of the Material Properties of Helium*, Salzgitter, Federal Republic of Germany: Safety Standards of the Nuclear Safety Standards Commission.
- KTA, 1981. *Reactor Core Design of High-Temperature Gas-Cooled Reactors, Part 3: Loss of Pressure through Friction in Pebble Bed Cores*, Salzgitter, Federal Republic of Germany: Safety Standards of the Nuclear Safety Standards Commission.
- KTA, 1983. *Reactor Core Design of High-Temperature Gas-Cooled Reactors, Part 2: Heat Transfer in Spherical Fuel Elements*, Salzgitter, Federal Republic of Germany: Safety Standards of the Nuclear Safety Standards Commission.
- KTA, 1984. *Reactor Core Design of High-Temperature Gas-Cooled Reactors, Part 4: Thermohydraulic Analytical Model for Stationary and Quasi-Stationary Conditions in Pebble Bed Cores*, Salzgitter, Federal Republic of Germany: Safety Standards of the Nuclear Safety Standards Commission.
- Kugeler, K., Nabielek, H. & Buckthorpe, D., 2017. *The High Temperature Gas-cooled Reactor: Safety considerations of the (V)HTR-Modul*. Luxembourg: European Atomic Energy Community.
- Kugeler, K. & Schulten, R., 1989. *High-temperature reactor development. Hochtemperaturreaktortechnik*. Berlin: Springer-Verlag.
- Lamarche, F. & Leroy, C., 1990. Evaluation of the volume of intersection of a sphere with a cylinder by elliptic integrals. *Comput. Phys. Commun.*, 59(2), pp. 359-369.

- Lange, M., 1995. *Experimente zur selbsttätigen abfuhr der nachwärme bei Hochtemperatur-Reaktoren: Planung, Vorbereitung und Ergebnisse.*, Aachen, Germany: Berichte des Forschungszentrums Jülich: Jül-3012.
- Lim, H. S. & No, H. C., 2006. GAMMA Multidimensional Multicomponent Mixture Analysis to Predict Air Ingress Phenomena in an HTGR. *Nuclear Science and Engineering*, 152(1), pp. 87-97.
- Li, Y. et al., 2015. Effect of wall structure on pebble stagnation behavior in pebble bed reactor. *Annals of Nuclear Energy*, Volume 80, pp. 195-202.
- Li, Y. & Ji, W., 2013. Pebble Flow and Coolant Flow Analysis Based on a Fully Coupled Multiphysics Model. *Nuclear Science and Engineering*, Volume 173, pp. 150-162.
- Luo, X., Li, X. & Yu, S., 2010. Nuclear graphite friction properties and the influence of friction properties on the pebble bed. *Nucl. Eng. Des.*, 240(10), p. 2674–2681.
- Luo, Y. et al., 2024. A novel contact thermal resistance model for heat transfer in granular systems: Leveraging the force-heat analogy. *International Journal of Heat and Mass Transfer*, Volume 232, p. 125919.
- Malan, A. G., Visser, C. J. & Meyer, J. P., 2006. *Modelling heat and fluid flow through packed beds - a density based vertex-centered methodology*. Johannesburg, South Africa, 3rd International Topical Meeting on High Temperature Reactor Technology (HTR2006).
- Mariani, N. J., Mazza, G. D., Martinex, O. M. & Barreto, G. F., 2000. Evaluation of Radial Voidage Profiles in Packed Beds of Low-Aspect Ratios. *Can. J. Chem. Eng.*, 78(6), pp. 1133-1137.
- Martin, H., 1978. Low Péclet Number Particle-to-Fluid Heat and Mass Transfer in Packed Beds. *Chem. Eng. Sci.*, 33(7), pp. 913-919.
- Mindlin, R. D. & Deresiewicz, H., 1953. Elastic Spheres in Contact Under Varying Oblique Forces. *ASME J. Appl. Mech.*, 20(3), pp. 327-344.
- Mitchell, M. N. & Polson, A. G., 2007. Assessment of the loads on a solid centre reflector of a Pebble Bed Reactor using DEM techniques. *Nuclear Engineering and Design*, Volume 237, pp. 1332-1340.
- M-Tech Industrial, 2008. *HTTU002-0016 Revision 2 High Temperature Test Unit (HTTU) Test Report for Nitrogen Natural Convection Tests*, Potchefstroom: M-Tech Industrial (Pty) Ltd..
- M-Tech Industrial, 2009a. *HTTU002-0037 Revision 2 High Temperature Test Unit (HTTU) Test Report for Nitrogen Forced Flow Isothermal Tests*, Potchefstroom: M-Tech Industrial (Pty) Ltd..
- M-Tech Industrial, 2009b. *HTTU002-0045 Revision 2 High Temperature Test Unit (HTTU) Test Report for Nitrogen Near Vacuum High Temperature (1200 °C) Tests*, Potchefstroom: M-Tech Industrial (Pty) Ltd..
- M-Tech Industrial, 2009c. *HTTU002-0053 Revision 2 High Temperature Test Unit (HTTU) Test Report for Helium Natural Convection Tests*, Potchefstroom: M-Tech Industrial (Pty) Ltd..
- M-Tech Industrial, 2009d. *HTTU002-0059 Revision 1 High Temperature Test Unit (HTTU) Test Report for Forced Convection High Temperature Tests*, Potchefstroom: M-Tech Industrial (Pty) Ltd..
- M-Tech Industrial, 2024. *Flownex Simulation Environment: Flownex Theory Manual*, Potchefstroom: M-Tech Industrial.
- Mueller, G. E., 1992. Radial void fraction distribution in randomly packed fixed beds of uniformly sized spheres in cylindrical containers. *Powder Technol.*, 72(3), pp. 269-275.
- Mueller, G. E., 2005. Numerically packing spheres in cylinders. *Powder Technol.*, 159(2), pp. 105-110.

- Mueller, G. E., 2010. Radial porosity in packed beds of spheres. *Powder Technol.*, 203(3), pp. 626-633.
- Mueller, G. E., 2012. A simple method for determining sphere packed bed radial porosity. *Powder Technol.*, Volume 229, pp. 90-96.
- NEA, 2013. *PBMR Coupled Neutronics/Thermal-hydraulics Transient Benchmark: The PBMR-400 Core Design - Volume 1: The Benchmark Definition*, Paris, France: OECD Publishing.
- NEK, 2024. *Nek5000: Open source, highly scalable and portable spectral element code*. [Online] Available at: <https://nek5000.mcs.anl.gov/> [Accessed 11 November 2024].
- Nicholls, D. R., 2017. *Advanced High Temperature Reactor Project – PBMR relaunch*. Cape Town, South Africa, Eskom.
- Novak, A., 2020. *Multiscale Thermal-Hydraulic Methods for Pebble Bed Reactors*, Berkeley, CA: University of California, Berkeley.
- Novak, A. J. et al., 2019. Validation of Pronghorn friction-dominated porous media thermal-hydraulics model with the SANA experiments. *Nucl. Eng. Des.*, Volume 350, pp. 182-194.
- Novak, A. J. et al., 2018. *Pronghorn: Porous media thermal-hydraulics for reactor applications*, s.l.: UC Berkeley.
- Nuclear Energy Agency (NEA), 2014. *Technology Roadmap Update for Generation IV Nuclear Energy Systems*, s.l.: OECD Nuclear Energy Agency.
- NWU, 2009. *Personal communication during a tour of the HTTU facility*. s.l.:s.n.
- Pebble Bed Modular Reactor SOC Ltd., 2016. *Letter 128884-1*, s.l.: s.n.
- Pebble Bed Modular Reactor SOC Ltd., 2017. *PBMR - Welcome*. [Online] Available at: <https://www.pbmr.co.za/index2.asp> [Accessed 16 March 2024].
- Peng, H.-R. & Sun, J., 2016. Investigation of Flow and Heat Transfer in the Pebble Bed of the High Temperature Gas-cooled Reactor. *Journal of Engineering Thermophysics*, 37(5), pp. 1076-1083.
- Pitso, L. M., 2011. *Characterisation of long range radiation heat transfer in packed pebble beds*, Potchefstroom: North-West University.
- Potgieter, M. C. & Du Toit, C. G., 2023. The porosity distribution in the HTTU annular packed bed of spheres. *Nuclear Engineering and Design*, Volume 402, p. 112124.
- Potgieter, M. C. & Du Toit, C. G., 2024. Analysis of forced convection in the HTTU experiment using numerical codes. *Nuclear Engineering and Technology*, 56(3), pp. 959-965.
- Potgieter, M. C., Du Toit, C. G. & Kruger, J. -H., 2016b. *The evaluation of 3D CFD approaches to model the flow and heat transfer inside an unstructured bed of uniform spheres*. Potchefstroom, South Africa, 10th South African Conference on Computational and Applied Mechanics (SACAM 2016).
- Potgieter, M. C., Du Toit, C. G. & Kruger, J.-. H., 2016a. *A fully integrated 3D CFD model of the flow and heat transfer in a packed bed reactor (Paper 188)*. Las Vegas, NV, USA, 8th International Topical Meeting on High Temperature Reactor Technology (HTR 2016).
- Preller, A. C. C., 2011. *Numerical modelling of flow through packed beds of uniform spheres*, Potchefstroom: North-West University.

- Reger, D., Merzari, E., Balestra, P. & Hassan, Y., 2024. Improving the modeling of near-wall interphase heat transfer in porous media models of Pebble Bed Reactors. *Nuclear Engineering and Design*, Volume 427, p. 113424.
- Reimann, J. et al., 2017. X-ray tomography investigations of mono-sized sphere packing structures in cylindrical containers. *Powder Technol.*, Volume 318, pp. 471-483.
- Reitsma, F., 2021. Pebble Bed Gas Cooled Reactors. In: E. Greenspan, ed. *Encyclopedia of Nuclear Energy*. Online: Elsevier, pp. 721-731.
- Ren, C. et al., 2017. Theoretical Analysis of Effective Thermal Conductivity for the Chinese HTR-PM Heat Transfer Test Facility. *Applied Sciences*, 7(1), p. 76.
- Reyneke, H. J., 2009. *Investigation into the velocity distribution through an annular packed bed*, Potchefstroom: North-West University.
- Reyneke, H. J. & Du Toit, C. G., 2010. *Modelling the Superficial Velocity Distribution Inside an Annular Packed Bed*. Pretoria, South Africa, 7th South African Conference on Computational and Applied Mechanics (SACAM10).
- Robold, R., 1982. Wärmetransport im Inneren und in der Randzone von Kugelschüttungen. *Berichte der Kernforschungsanlage Jülich*.
- Rodríguez, A. G. et al., 2021. An integral 3D full-scale steady-state thermohydraulic calculation of the high temperature pebble bed gas-cooled reactor HTR-10. *Nucl. Eng. Des.*, Volume 373, p. 111011.
- Rosatom, 2023. *Rosatom Newsletter #270*. [Online]
Available at: <https://rosatomnewsletter.com/2023/10/30/high-temperature-gas-cooled-reactor/>
[Accessed 29 October 2024].
- Rousseau, P. G., Du Toit, C. G. & Landman, W. A., 2006. Validation of a transient thermal-fluid systems CFD model for a packed bed high temperature gas-cooled nuclear reactor. *Nuclear Engineering and Design*, 236(5-6), pp. 555-564.
- Rousseau, P. G., Du Toit, C. G. & Van Antwerpen, H. J., 2019. CFD and systems thermal-hydraulic analysis in the design and safety assessment of high-temperature reactors. In: J. B. Joshi & A. K. Nayak, eds. *Advances of Computational Fluid Dynamics in Nuclear Reactor Design and Safety Assessment*. Online: Woodhead Publishing, pp. 755-800.
- Rousseau, P. G., Du Toit, C. G., Van Antwerpen, W. & Van Antwerpen, H. J., 2014. Separate effects tests to determine the effective thermal conductivity in the PBMR HTTU test facility. *Nuclear Engineering and Design*, Volume 271, pp. 444-458.
- Rousseau, P. G. & Van Staden, M., 2008. Introduction to the PBMR heat transfer test facility. *Nucl. Eng. Des.*, 238(11), pp. 3060-3072.
- Rycroft, C. H., Dehbi, A., Lind, T. & Güntay, S., 2013. Granular flow in pebble-bed nuclear reactors: Scaling, dust generation, and stress,. *Nuclear Engineering and Design*, Volume 265, pp. 69-84.
- Sandia National Laboratories, 2002. *Verification and Validation in Computational Fluid Dynamics*, Albuquerque, New Mexico: Sandia National Laboratories.
- Scari, M. E. et al., 2016. HTR steady state and transient thermal analyses. *International Journal of Hydrogen Energy*, 41(17), pp. 7192-7196.

- Sederman, A. J., Alexander, P. & Gladden, L. F., 2001. Structure of packed beds probed by Magnetic Resonance Imaging. *Powder Technol.*, 117(3), pp. 255-269.
- Seker, V. & Downar, T. J., 2007. *Multiphysics Methods Development for High Temperature Gas Cooled Reactor Analysis*. Istanbul, Türkiye, International Conference on Emerging Nuclear Energy Systems (ICENES-2007).
- Shams, A., Roelofs, F., Komen, E. M. J. & Baglietto, E., 2014. Large eddy simulation of a randomly stacked nuclear pebble bed. *Computers & Fluids*, Volume 96, pp. 302-321.
- Shaver, D. R. et al., 2023. Demonstration of RANS models with wall functions in the spectral element code Nek5000. *Nuclear Engineering and Design*, Volume 408, p. 112302.
- Siemens, 2023. *Simcenter STAR-CCM+ User Guide Documentation Version 2310*, Digital: Siemens Digital Industries Software.
- Siemens, 2024. *Simcenter STAR-CCM+ CFD software*. [Online]
Available at: <https://plm.sw.siemens.com/en-US/simcenter/fluids-thermal-simulation/star-ccm/>
[Accessed 11 November 2024].
- Span, R. et al., 2000. A Reference Equation of State for the Thermodynamic Properties of Nitrogen for Temperatures from 63.151 to 1000 K and Pressures to 2200 MPa. *Journal of Physical and Chemical Reference Data*, 29(6), pp. 1361-1433.
- Stöcker, B. & Nießen, H.-F., 1997. *Data Sets of the SANA Experiment 1994-1996*, Jülich, Germany: Forschungszentrum Jülich GmbH.
- Suikkanen, H., Rintala, V. & Kyrki-Rajamäki, R., 2014. *Development of a Coupled Multi-Physics Code System for Pebble Bed Reactor Core Modeling*. Weihai, China, Proceedings of the HTR 2014.
- Suikkanen, H., Ritvanen, J., Jalali, P. & Kyrki-Rajamäki, R., 2014. Discrete element modelling of pebble packing in pebble bed reactors. *Nucl. Eng. Des.*, Volume 273, pp. 24-32.
- The OpenFOAM Foundation, 2024. *OpenFOAM v12 User Guide*. [Online]
Available at: <https://doc.cfd.direct/openfoam/user-guide-v12/index>
[Accessed 11 November 2024].
- Theuerkauf, J., Witt, P. & Schwesig, D., 2006. Analysis of particle porosity distribution in fixed beds using the discrete element method. *Powder Technol.*, 165(2), pp. 92-99.
- Tsory, T., Ben-Jacob, N., Brosh, T. & Levy, A., 2013. Thermal DEM-CFD modeling and simulation of heat transfer through packed bed. *Powder Technology*, Volume 244, pp. 52-60.
- Vafai, K., 2005. *Handbook of Porous Media*. 2nd ed. Boca Raton, FL: Taylor & Francis Group, LLC.
- Van Antwerpen, W., 2009. *Modelling the effective thermal conductivity in the near-wall region of a packed pebble bed*, Potchefstroom: North-West University.
- Van Antwerpen, W., du Toit, C. G. & Rousseau, P. G., 2010. A review of correlations to model the packing structure and effective thermal conductivity in packed beds of mono-sized spherical particles. *Nucl. Eng. Des.*, 240(7), pp. 1803-1818.
- Van Antwerpen, W., Rousseau, P. G. & du Toit, C. G., 2012. Multi-sphere Unit Cell model to calculate the effective thermal conductivity in packed pebble beds of mono-sized spheres. *Nucl. Eng. Des.*, Volume 247, pp. 183-201.
- Van der Merwe, W. J. S., 2014. *Analysis of flow through cylindrical packed beds with small cylinder diameter to particle diameter ratios*, Potchefstroom: North-West University.

- Van der Walt, S., 2020. *The zonal approach applied to the simulation of the radiative heat transfer in a packed pebble bed*, Potchefstroom: North-West University.
- Van Dijk, V., 2008. *Radial void fraction measurement of a randomly packed pebble-bed*, Delft, The Netherlands: Delft University of Technology.
- Van Loggerenberg, P. J., 2020. *Analysis of the pressure drop through structured packed beds*, Potchefstroom: North-West University.
- Van Staden, M. P., Neykov, B. & Mulder, E., 2018. *Explicit Modelling of Randomly Packed Pebble Bed Using RANS CFD Modelling*. Warsaw, Poland, HTR 2018-167.
- Venter, P. J. & Mitchell, M. N., 2007. Integrated design approach of the pebble BeD modular reactor using models. *Nuclear Engineering and Design*, 237(12-13), pp. 1341-1353.
- Vermaak, H. J., 2019. *CFD analysis of thermal dispersion in a structured pebble bed*, Potchefstroom: North-West University.
- Von Seckendorff, J. et al., 2021. Experimental and numerical analysis of void structure in random packed beds of spheres. *Powder Technol.*, Volume 380, p. 613-628.
- Von Seckendorff, J. & Hinrichsen, O., 2021. Review on the structure of random packed-beds. *Can. J. Chem. Eng.*, Volume 99, pp. S703-S733.
- Vortmeyer, D. & Schuster, J., 1983. Evaluation of steady flow profiles in rectangular and circular packed beds by a variational method. *Chem. Eng. Sci.*, 38(10), pp. 1691-1699.
- Wang, X., Zheng, J. & Chen, H., 2016. A prediction model for the effective thermal conductivity of mono-sized pebble beds. *Fusion Engineering and Design*, Volume 103, pp. 136-151.
- Wassgren, C. & Sarkar, A., 2008. *PSL DEM Lecture 06: Introduction to Soft-Particle DEM and Normal Contact Force Models - Part I*. [Online]
Available at: <https://pharmahub.org/resources/122>
- Wen, D. & Ding, Y., 2006. Heat transfer of gas flow through a packed bed. *Chemical Engineering Science*, 61(11), pp. 3532-3542.
- Weng, J. et al., 2023. Numerical determination of fluid-to-particle mass and heat transfer coefficients in packed bed reactors. *AIChE Journal*, 69(5), p. e17980.
- White, S. M. & Tien, C. L., 1987. Analysis of flow channeling near the wall in packed beds. *Wärme-Stoffübertragung*, 21(5), p. 291-296.
- Wolf, L., Scherer, W., Giesser, W. & Feltes, W., 1990. High temperature reactor core physics and reactor dynamics. *Nuclear Engineering and Design*, 121(2), pp. 227-240.
- World Nuclear Association, 2024. *Nuclear Energy and Sustainable Development*. [Online]
Available at: <https://world-nuclear.org/information-library/energy-and-the-environment/nuclear-energy-and-sustainable-development>
[Accessed 7 November 2024].
- World Nuclear News, 2022. *DOE marks milestone as Xe-100 basic design completed*. [Online]
Available at: <https://www.world-nuclear-news.org/Articles/DOE-marks-milestone-as-Xe-100-basic-design-complete>
[Accessed 11 November 2024].

- Wu, C. Y., Ferng, Y. M., Chieng, C. C. & Liu, C. C., 2010. Investigating the advantages and disadvantages of realistic approach and porous approach for closely packed pebbles in CFD simulation. *Nuclear Engineering and Design*, 240(5), pp. 1151-1159.
- Wu, H. et al., 2017. Numerical simulation of heat transfer in packed pebble beds: CFD-DEM coupled with particle thermal radiation. *International Journal of Heat and Mass Transfer*, Volume 110, pp. 393-405.
- Wu, Z., Lin, D. & Zhong, D., 2002. The design features of the HTR-10. *Nuclear Engineering and Design*, Volume 218, pp. 25-32.
- Xu, Y., 2002. *The HTR-10 project and its further development*. Institute of Nuclear Energy Technology, Tsinghua University, Beijing, HTR-2002: Proceedings of the conference on high temperature reactors.
- Yang, J., Wu, J., Zhou, L. & Wang, Q., 2016. Computational study of fluid flow and heat transfer in composite packed beds of spheres with low tube to particle diameter ratio. *Nuclear Engineering and Design*, Volume 300, pp. 85-96.
- Yang, X., Gui, N., Tu, J. & Jiang, S., 2014. 3D DEM simulation and analysis of void fraction distribution in a pebble bed high temperature reactor. *Nucl. Eng. Des.*, Volume 270, pp. 404-411.
- Zehner, P. & Schlünder, E. U., 1970. Thermal conductivity of granular materials at moderate temperatures. *Chemie Ingr. Tech.*, Volume 42, pp. 933-941.
- Zenner, A. et al., 2019. Effective heat transfers in packed bed: Experimental and model investigation. *Chemical Engineering Science*, Volume 201.
- Zhang, Z. et al., 2016. The Shandong Shidao Bay 200 MWe High-Temperature Gas-Cooled Reactor Pebble-Bed Module (HTR-PM) Demonstration Power Plant: An Engineering and Technological Innovation. *Engineering*, 2(1), pp. 112-118.
- Zhang, Z. & Yu, S., 2002. Future HTGR developments in China after the criticality of the HTR-10. *Nuclear Engineering and Design*, 218(1-3), pp. 249-257.
- Zhang, Z. et al., 2024. Pebble flow in the HTR-PM reactor core by GPU-DEM simulation: Effect of friction. *Nuclear Engineering and Technology*, 56(9), pp. 3835-3850.
- Zhao, X., Montgomery, T. & Zhang, S., 2015. Modeling stationary and moving pebbles in a pebble bed reactor. *Annals of Nuclear Energy*, Volume 80, pp. 52-61.
- Zheng, Y. et al., 2012. Thermal hydraulic analysis of a pebble-bed modular high temperature gas-cooled reactor with ATTICA3D and THERMIX codes. *Nuclear Engineering and Design*, Volume 246, pp. 286-297.
- Zou, L. et al., 2024. Thermal Fluid Modeling Approaches in SAM for High Temperature Gas-Cooled Reactor Applications. *Nuclear Technology*, pp. 1-18.
- Zou, L., Hu, G., O'Grady, D. & Hu, R., 2022. Explicit modeling of pebble temperature in the porous-media model for pebble-bed reactors. *Progress in Nuclear Energy*, Volume 146, p. 104175.
- Zou, L. et al., 2018. *Pronghorn: A Porous Media Thermal-Hydraulics Core Simulator and its Validation with the SANA Experiments*, Idaho Falls, ID: Idaho National Laboratory.
- Zou, Q. et al., 2023. A GPU-based DEM model for the pebble flow study in packed bed: Simulation scheme and validation. *Powder Technology*, Volume 422, p. 118441.
- Zou, Q., Zhang, Z., Gui, N. & Yang, X., 2024. Numerical study of the particle-scale heat transfer in the HTR-PM pebble bed based on GPU-DEM. *International Journal of Thermal Sciences*, Volume 205, p. 109300.

APPENDICES

A. HTTU TEST DATA

The experimental data of the 140 kW 1 kg/s forced convective test case is provided here for reference. Temperature values are taken as the average value from the two tests with the least uncertainty. The Level B, C and D positions are located at 120 ± 30 mm, 600 ± 15 and 960 ± 15 mm, respectively.

Radial Position [m]	0.3	0.3	0.3385	0.401667	0.475667	0.524333
Level B – avg. T [C]	756.44	717.34	488.07	316.44	164.06	101.59
Level C – avg. T [C]	884.84	864.60	789.46	632.44	485.59	323.69
Level D – avg. T [C]	1003.48	1002.27	725.92	735.12	574.30	409.78

Radial Position [m]	0.553	0.636	0.706333	0.761333	0.819	0.874667
Level B – avg. T [C]	n/c	40.07	32.14	29.25	28.06	27.26
Level C – avg. T [C]	225.59	127.77	83.66	50.33	35.97	35.70
Level D – avg. T [C]	295.73	199.81	117.13	69.39	50.80	37.52

Radial Position [m]	0.941333	1.001	1.045333	1.101667	1.15	1.15
Level B – avg. T [C]	29.78	31.66	33.02	31.68	27.36	27.83
Level C – avg. T [C]	28.72	35.85	32.84	33.32	27.92	27.87
Level D – avg. T [C]	30.90	35.22	30.17	29.39	33.04	32.35

B. USER DEFINED FUNCTIONS

This appendix lists the various UDFs with their formula and in code as utilised in simulation.

B-1. Discrete approach

B-1.1. Inner and outer reflector graphite thermal conductivity

The thermal conductivity in [W/m·K] of the inner and outer reflector graphite was used as a curve fitted function on the data from the manufacturer UCAR as a function of temperature in [K]. The function is piecewise-defined with an upper and lower limit in order to prevent an unrealistic shape as the curve-fitted function deviated significantly from the real values where it falls outside of the data range.

Definition:

$$k_{UCAR}(T) = \begin{cases} 173 & \text{if } T < 300 \\ 2.59 \times 10^{-5} \cdot T^2 - 0.1345 \cdot T + 211.18 & \text{if } 300 \leq T \leq 1500 \\ 67 & \text{if } T > 1500 \end{cases}$$

Java code used in Star-CCM+:

```
($ {Temperature}<300) ? 173 : ($ {Temperature}>1500) ? 67 : (2.5909856E-5*pow($ {Temperature},2) -0.13450253*$ {Temperature} + 211.1834)
```

B-1.2. Pebble thermal conductivity (Appendix C, from SGL)

The thermal conductivity in [W/m·K] of pebble graphite was defined as a function of temperature in [K] obtained from the curve fit of the conductivity data from the manufacturer SGL. It should be noted that the pebbles were manufactured by turning from extruded bar stock and therefore the thermal conductivity is anisotropic. As it is impossible to determine the actual orientation of the pebbles, the arithmetic average was taken at each datapoint of the x and y-direction values shown in the graph in Appendix C. The function is piecewise-defined with an upper and lower limit in order to prevent an unrealistic shape as the curve-fitted function deviated significantly from the real values where it falls outside of the data range.

Definition:

$$k_{SGL}(T) = \begin{cases} 158 & \text{if } T < 300 \\ 8.1989 \times 10^{-14} \cdot T^5 - 3.64 \times 10^{-10} \cdot T^4 + 5.457 \times 10^{-7} \cdot T^3 - 2.228 \times 10^{-4} \cdot T^2 - 0.19576 \cdot T + 224.94 & \text{if } 300 \leq T \leq 1586 \\ 50.345 & \text{if } T > 1586 \end{cases}$$

Java code used in Star-CCM+:

```
($Temperature<300) ? 158 : ($Temperature<1586) ? (8.198947E-14)*pow($Temperature,5) -3.640602E-10*pow($Temperature,4) +5.457479E-7*pow($Temperature,3) -2.228729E-4*pow($Temperature,2) -0.1957602*($Temperature)+224.9443) : 50.345
```

B-1.3. Pebble contact resistances (De Beer, 2021)

In the solid domain each pebble was defined as a unique solid sphere oversized by 0.5 % (for an absolute diameter of 60.3 mm). The overlap is used to allow easy definition of contact interfaces.

In the energy solver definition of the contacts, a thermal resistance is imposed equal to the effective thermal conductivity obtained experimentally by (De Beer, *et al.*, 2018) in the Near-Wall Thermal Conductivity Test Facility (NWTCTF) where a structured bed allowed an accurate derivation of the solid contact conductivity.

Definition:

$$R_{cont}(T) = \begin{cases} 5.57 \times 10^{-5} & \text{if } T < 300 \\ 1.623 \times 10^{-8} \cdot T + 6.059 \times 10^{-5} & \text{if } 300 \leq T \leq 1500 \\ 3.624 \times 10^{-5} & \text{if } T > 1500 \end{cases}$$

Java code used in Star-CCM+:

```
${Temperature}<300 ? 5.57E-5 : ${Temperature}>1500 ? 3.624E-5 : -1.623596E-8*${Temperature} +6.059437E-5
```

B-1.4. Nitrogen gas density (Kleiber & Joh, 2010)

The nitrogen density is prescribed as a real gas according to the Van der Waals equation of state.

Another recommended reference for fluid properties of Nitrogen is: Span, *et al.* (2000)

B-1.5. Nitrogen gas specific heat (Kleiber & Joh, 2010)

Although not used in steady-state calculations, the nitrogen c_p value was also user-defined as it is used in the Prandtl number calculation.

Definition:

$$c_{p,N_2}(T) = \begin{cases} 1038.97 & \text{if } T < 272 \\ 296.8 \left[\begin{aligned} & 3.516 + (2.8021 - 3.516) \left(\frac{T}{432 + T} \right)^2 \\ & 1 - \frac{432}{432 + T} \left(\begin{aligned} & -4.192 + 42 \left(\frac{T}{432 + T} \right) \\ & -114 \left(\frac{T}{432 + T} \right)^2 + 111 \left(\frac{T}{432 + T} \right)^3 \end{aligned} \right) \end{aligned} \right] & \text{if } 272 \leq T \leq 2423 \\ 1285.572 & \text{if } T > 2423 \end{cases}$$

Java code used in Star-CCM+:

```
{Temperature}<272 ? 1038.97 : {Temperature}<2422.5 ? (296.8*(3.516 +(2.8021 -
3.516)*pow(({Temperature}/(432.2027 + {Temperature})),2)*(1 -
(432.2027/(432.2027 + {Temperature}))*(-4.1924
+42.0153*({Temperature}/(432.2027 +{Temperature}))) -
114.25*pow(({Temperature}/(432.2027 +{Temperature})),2)
+111.1019*pow(({Temperature}/(432.2027 +{Temperature})),3)))) : 1285.572
```

B-1.6. Nitrogen gas dynamic viscosity (Kleiber & Joh, 2010)

Definition:

$$\mu_{N_2}(T) = \begin{cases} 6.73 \times 10^{-18} \cdot T^4 + 3.23 \times 10^{-14} \cdot T^3 - 5.9 \times 10^{-11} \cdot T^2 \\ + 7.4 \times 10^{-8} \cdot T - 1.02 \times 10^{-7} & \text{if } T \leq 2167 \\ 6.5 \times 10^{-5} & \text{if } T > 2167 \end{cases}$$

Java code used in Star-CCM+:

```
{Temperature}<2167 ? (-1.02E-7 +7.4785E-8*{Temperature} -5.9037E-
11*pow({Temperature},2) + 3.23E-14*pow({Temperature},3) -6.73E-
18*pow({Temperature},4)) : 6.5E-5
```

B-1.7. Nitrogen gas thermal conductivity (Kleiber & Joh, 2010)

Definition:

$$k_{N_2}(T) = \begin{cases} -1.33 \times 10^{-15} \cdot T^4 + 1.01 \times 10^{-11} \cdot T^3 - 6.065 \times 10^{-8} \cdot T^2 \\ + 1.01 \times 10^{-4} \cdot T - 1.33 \times 10^{-4} & \text{if } T \leq 2380 \\ 0.122 & \text{if } T > 2380 \end{cases}$$

Java code used in Star-CCM+:

```
${Temperature}<2380 ? (-1.33E-4+1.01E-4*${Temperature}-6.065E-8*pow(${Temperature},2) +3.361E11*pow(${Temperature},3) -7.1E-15*pow(${Temperature},4)) : 0.122
```

B-1.8. Nitrogen gas turbulent Prandtl number

When the value of the nitrogen Prandtl number is not specified as a constant, it needs to be defined as a user field function. For this reason, the Prandtl number was defined as follows and referenced the user-defined functions for all three variables in its definition:

$$\text{Pr} = \frac{c_p \cdot \mu}{k}$$

As the three variables are all functions of temperature, the Prandtl number could also be defined as a stand-alone function only dependent on temperature.

Java code used in Star-CCM+:

```
${SpecificHeat}*${DynamicViscosity}/${ThermalConductivity}
```

B-1.9. Mass flow boundary condition

A ramp of the steady-state inlet mass flow boundary condition as a function of the iteration number

Definition:

$$\dot{m}(i) = \begin{cases} 1.25 \times 10^{-5} \cdot i + 6.25 \times 10^{-3} & \text{iteration} < 4500 \\ 0.0625 & \text{iteration} \geq 4500 \end{cases}$$

Java code used in Star-CCM+:

```
${Iteration}<4500 ? 1.25E-5*${Iteration}+6.25E-3 : 6.25E-2
```

B-1.10. Heat source boundary condition

A ramp of the steady-state heat input boundary condition as function of the iteration

Definition:

$$\dot{Q}(i) = \begin{cases} 0 & \text{iteration} < 1000 \\ 1.1 \cdot i - 1100 & 1000 \leq \text{iteration} \leq 8500 \\ 8250 & \text{iteration} > 8500 \end{cases}$$

Java code used in Star-CCM+:

```
(${Iteration}<8500 && ${Iteration}<1000) ? 0 : (${Iteration}<8500 &&
${Iteration}>1000) ? 1.1*${Iteration}-1100 : 8250
```

B-2. Porous approach

Refer to the KTA standards for the formulae used (KTA, 1981)

B-2.1. Pressure drop

B-2.1.1. Viscous term

Definition:

$$\frac{160 \cdot \mu \cdot (1 - \varepsilon)^2}{\varepsilon^3 \cdot d_p^2}$$

Java code used in Star-CCM+:

```
160.0*$DynamicViscosity*pow((1-$BedPorosity),2)/(pow($BedPorosity,3)*pow($BedSphereDiameter,2))
```

B-2.1.2. Inertial term

Definition:

$$3 \cdot \rho \cdot \frac{(1 - \varepsilon)}{\text{Re}^{0.1}} \cdot \varepsilon^3 \cdot d_p$$

Java code used in Star-CCM+:

```
(3*${Density}*(1-$BedPorosity))/(pow(${ReynoldsNumber},0.1)*pow(${BedPorosity},3)*$BedSphereDiameter)
```

B-2.2. Interaction area density

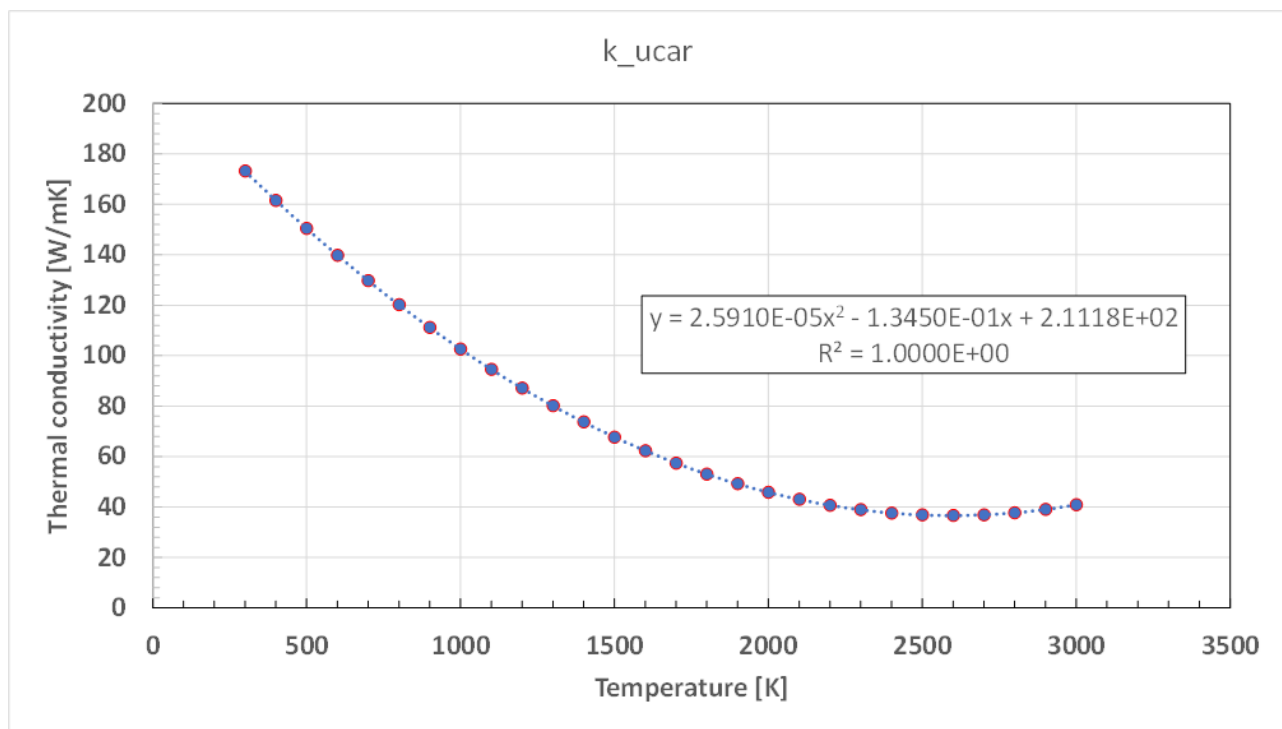
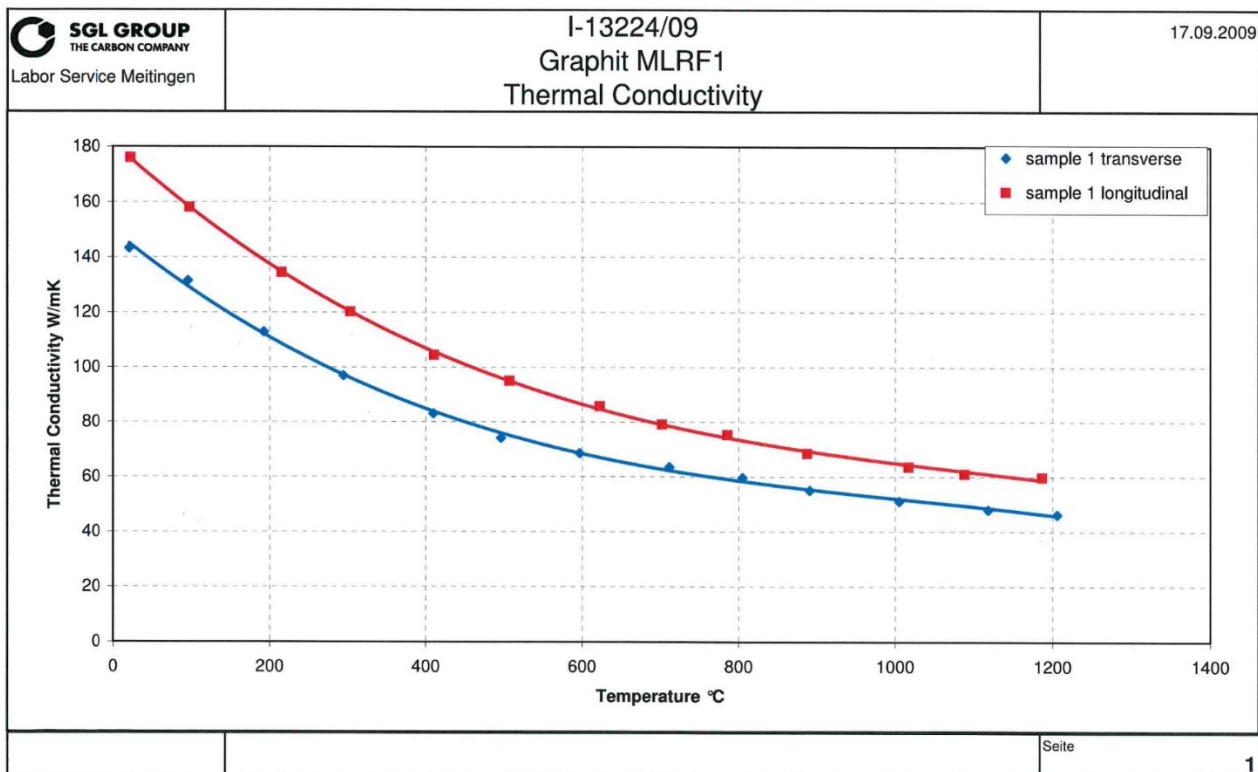
Defined as it relates to porosity for the case of perfect spheres of equal diameter:

$$100 \cdot (1 - \varepsilon)$$

Java code used in Star-CCM+:

```
100*(1-$BedPorosity)
```

C. THERMAL CONDUCTIVITY



D. SUMMARY OF KTA CORRELATIONS

KTA Safety Standards for the analytical investigation of a pebble bed HTGR

D-1. KTA 3102.1 – Calculation of the Fluid Properties of Helium

The pressure range is 1 bar to 100 bar and the temperature range is 20 °C to 1500 °C

Density

$$\rho = 48.14 \cdot \frac{p}{T} \left(1 + 0.4446 \cdot \frac{p}{T^{1.2}} \right)^{-1} \text{ in } \left[\frac{\text{kg}}{\text{m}^3} \right]$$

$$\sigma_\rho = 0.03 \cdot \sqrt{p} \text{ in } [\%]$$

Specific heat

$$c_p = 5195 \text{ in } \left[\frac{\text{J}}{\text{kg} \cdot \text{K}} \right] \text{ for constant pressure}$$

$$\sigma_{c_p} = 0.05 \cdot p^{\left(0.6 - 0.1 \cdot \frac{T}{273.16} \right)} \text{ in } [\%]$$

Dynamic viscosity

$$\mu = 3.674 \times 10^{-7} \cdot T^{0.7} \text{ in } [\text{Pa} \cdot \text{s}]$$

$$\sigma_\mu = 0.0015 \cdot T \text{ in } [\%]$$

Thermal conductivity

$$k = 2.682 \times 10^{-3} \left(1 + 1.123 \times 10^{-3} \cdot p \right) \cdot T^{0.71 \left(1 - 2 \times 10^{-4} \cdot p \right)} \text{ in } \left[\frac{\text{W}}{\text{m} \cdot \text{K}} \right]$$

$$\sigma_k = 0.0035 \cdot T \text{ in } [\%]$$

D-2. KTA 3102.2 – Heat Transfer in Spherical Fuel Elements

Range of Reynolds number $100 < Re < 10^5$

Porosity of the bed $0.36 < \varepsilon < 0.42$

Diameter ratio $D/d > 20$

Height of the bed $H > 4 d$

Convective heat transfer from pebbles to gas flow

$$\dot{Q} = \alpha \cdot A_K (T_K - T_G)$$

Calculation of the convective heat transfer coefficient

$$\alpha = \frac{Nu \cdot \lambda}{d}$$

Correlation for Nusselt number as function of porosity

$$Nu = 1.27 \frac{Pr^{1/3}}{\varepsilon^{1.18}} Re^{0.36} + 0.033 \frac{Pr^{1/2}}{\varepsilon^{1.07}} Re^{0.86}$$

The Reynolds number for the whole bed

$$Re = \frac{\dot{m} \cdot d}{A \cdot \mu}$$

D-3. KTA 3102.3 – Loss of Pressure through Friction in Pebble Bed Cores

Range of Reynolds number $10 < Re / (1 - \varepsilon) < 10^5$

Porosity of the bed $0.36 < \varepsilon < 0.42$

Diameter ratio Subject to limiting curve (refer to standard)

Height of the bed $H > 5 d$

$$\frac{\Delta p}{\Delta H} = \Psi \cdot \frac{1 - \varepsilon}{\varepsilon^3} \cdot \frac{1}{d} \cdot \frac{1}{2\rho} \cdot \left(\frac{\dot{m}}{A} \right)^2$$

$$\Psi = \frac{320}{\left(\frac{Re}{1 - \varepsilon} \right)} + \frac{6}{\left(\frac{Re}{1 - \varepsilon} \right)^{0.1}}$$

End of Appendices



The porosity distribution in the HTTU annular packed bed of spheres

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Annular packed bed
Axial porosity
Radial porosity
Porosity contours
Regional porosity

ABSTRACT

In this paper a comprehensive analysis of the porosity of the annular packed bed of the High Temperature Test Unit (HTTU) is presented. The annular packed bed is generated using a Discrete Element Method (DEM) approach. Semi-analytical methods are then used to analyse the porosity. The quality and representativity of the packed bed are established by evaluating the overlaps between spheres and spheres and walls and comparing the axial and radial variations in porosity with available experimental and numerical data. The angular and radial variation of selected sphere layers in the bottom near-wall region was studied revealing how the spheres in the axial layers and radial rings are staggered with respect to each other. The analysis of the radial variation in porosity also included the standard deviation and the skewness of the angular porosity at each radial position. An analysis of the radial porosity of the layers revealed that only first layer next to the bottom is markedly affected by the bottom wall. The interference between the oscillatory porosity variations perpendicular to the inner, outer, and bottom walls of the annular packed bed is demonstrated by the plot of the variation in porosity on an axi-symmetric r - z plane. The annular packed bed is also divided into 20 regions and the average porosity and the standard deviation of the porosity for each region is provided.

1. Introduction

Packed beds are prevalent in several industries, such as chemical processing and the food industry (Kolev, 2006) where applications are mainly focussed on separation and heat transfer processes. In the nuclear industry, several reactor designs have been based around a packed bed core design consisting of equal sized spheres (IAEA, 2013). The flow, pressure drop and heat transfer characteristics of a packed bed are dependent on the packing structure (Kugeler and Schulten, 1989; KTA, 1983; Rodríguez et al., 2021). The most influential characteristic of the porous structure is the porosity (Suikkanen et al., 2014; Von Seckendorff et al., 2021). A proper understanding of the porosity and how it affects the phenomena that determine the performance of the packed bed reactor is therefore required (Novak et al., 2019).

Many physical experiments that were performed to determine the porosity of packed beds have been reported. Destructive approaches (Benenatti and Brosilow, 1962; Goodling et al., 1983) and non-destructive approaches (Giese et al., 1998; Guo et al., 2017) have been employed to determine the porosity directly. Imaging methods have also been widely used to determine the porosity. The most notable are X-ray radiography (Mueller, 1992), X-ray computed tomography (Reimann et al., 2017; Von Seckendorff et al., 2021), gamma ray computed

tomography (Auwerda et al., 2010; Al Falahi and Al-Dahhan, 2016) and magnetic resonance imaging (Sederman et al., 2001). The variation in porosity was either determined directly from the images (Reimann et al., 2017; Al Falahi and Al-Dahhan, 2016; Sederman et al., 2001), or else the coordinates of the centres of the spheres (Mueller, 1992; Reimann et al., 2017; Von Seckendorff et al., 2021) were determined by analysing the images. Packing algorithms (Mueller, 2005; Jerier et al., 2010) and the Discrete Element Method (DEM) (Theuerkauf et al., 2006; Suikkanen et al., 2014) have been used to generate packed beds numerically. The coordinates of the spheres can be obtained directly from these methods. The variation in porosity can then be calculated numerically using volume-based methodologies (Lamarche and Leroy, 1990; Govindarao et al., 1990; Mueller, 1992), area-based methods (Mariani et al., 2000; Du Toit, 2002, 2019b; Mueller, 2010), and line-based methods (Mueller, 2012; Feng et al., 2021; Bester and Du Toit, 2022).

Analysis of the experimental and the numerical data have shown that there is a marked influence on the packing structure exercised by the wall and the ratio between the cylinder diameter and the sphere diameter, or aspect ratio. It was observed that the porosity varies in a damped oscillatory manner from a value of one at the wall to a bulk value some distance from the wall depending on the aspect ratio (Benenatti and Brosilow, 1962; Goodling et al., 1983; Giese et al., 1998). Empirical correlations having an exponential variation, such as by Vortmeyer and

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Original Article

Analysis of forced convection in the HTTU experiment using numerical codes

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ABSTRACT

The High Temperature Test Unit (HTTU) was an experimental set-up to conduct separate and integral effects tests of the Pebble Bed Modular Reactor (PBMR) core. The annular core consisted of a randomly packed bed of uniform spheres. Natural convection tests using both nitrogen and helium, and forced convection tests using nitrogen, were conducted. The maximum material temperature achieved during forced convection testing was 1200 °C. This paper presents the numerical analysis of the flow and temperature distribution for a forced convection test using 3D CFD as well as a 1D systems-CFD computer code. Several modelling approaches are possible, ranging from a fully explicit to a semi-implicit method that relies on correlations of their associated phenomena. For the comparison between codes, the analysis was performed using a porous media approach, where the conduction and radiative heat transfer were lumped together as an effective thermal conductivity and the convective heat transfer was correlated between the solid and gas phases. The results from both codes were validated against the experimental measurements. Favourable results were obtained, in particular by the systems-CFD code with minimal computational and time requirements.

1. Introduction

Constructed between 2006 and 2007, the High Temperature Test Unit (HTTU) was an experimental set-up to conduct separate and integral effects tests of the Pebble Bed Modular Reactor (PBMR) core in an annular configuration [1].

The HTTU was one of several experiments [2,3] that were a part of the High Temperature Test Facility (HTTF) which was hosted by the North-West University in South Africa and funded by PBMR (Pty) Ltd. These experiments, as well as the Pebble Bed Micro Model (PBMM), were applied towards the Verification & Validation (V&V) qualification testing [4] for licensing of the PBMR design.

The annular core of the HTTU experiment consisted of a randomly packed bed of approximately 25,000 uniform graphite spheres [5], not containing any fissile material. Firstly, for integral effects tests the core had two configurations: (i) forced convection with an open bed allowing flow to pass upwards through and exit the core, and (ii) natural convection with a closed bed to limit the temperatures of the support structures and allowing only natural convection to take place in the bed.

As part of the integral effects test runs, both natural convection tests using nitrogen and helium, and forced convection tests using nitrogen

were conducted. The maximum temperature obtained during natural and forced convection, as well as near-vacuum testing, was 1200 °C.

In order to determine the effective thermal conductivity of the bed through separate effects tests, the experiment was also run under near-vacuum high temperature conditions. The results from the latter tests are described in detail by Rousseau et al. [2].

In the interest of brevity and page limitations, only a brief literature overview is provided here. In previous validation studies the natural convection experiments performed in the SANA experiment [6] were simulated using either a 3D CFD approach [7,8] or a system 1D component network approach [9,10]. The predicted temperature distributions were compared with the experimentally measured temperatures. In all the simulation cases the packed bed was considered as a porous medium.

This study presents the numerical analysis of the flow and temperature distribution in the HTTU under forced convection conditions, using both a 3D CFD and a 1D systems-CFD computer code, and a comparison of the results from both methodologies with the experimental measurements.

Several modelling approaches are possible with the numerical techniques available: from a fully explicit numerical solution to semi-

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NON SCHOLAE SED VITAE DISCIMUS

– Seneca, *Epistulae Morales ad Lucilium* VII.8

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