Investigation into different 1D/3D thermal fluid co-simulation methodologies as applied to HTR system configurations

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Thesis accepted in fulfilment of the requirements for the degree Doctor of Philosophy in Engineering in Nuclear Engineering at the North-West University

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The truth is I’m… I’m not an exceptional person, you know.

Nothing interesting, really ever happens to me, I am massively flawed, and I think I’m quite forgettable if I’m being 100% honest, and this isn’t a bit at the end of an era where I get on the cross, I’m like “*love me on the way out the door*”, it’s not that, it’s just that I don’t think like on a scale of one to memorable, I’m not that memorable. I’m not on like the Saint Paul sort of scale; Not on the Louis C.K. or Hemingway scale certainly, you know? But if I tell a great story, maybe people will remember that instead. Remember the card trick and just pretend that they don’t know how it’s done, you know?

But must we leave a legacy?

Must we make an impact?

Do we have to leave a footprint?

Is it okay to just settle?... Seek Safety? Nest? …You know?

Or must we constantly shake our lives up? Or suffer the indiscriminate cruelty of having it shaken against our will. Must we try to carve a path through the tall grass, feeling as though no one has ever felt how we feel? Terrified at what may be lurking low in the grass on either side of us, but just pressing ever onwards with that Palaeolithic instinct deep within our chromosomes that the only way is forward.

That you have to keep going!

That eventually you’ll stumble upon the edge of the field, hitch a ride from a passing car, and meet up with the rest of the gang for tea and sandwiches at the old town hall…

sighs

Do we feel like the path that we are carving through the grass is all our own? Only to finally float above the field with the sweet relief of expiration and realize that the field is insignificantly minuscule in size and that there is only one path through the grass. The exact same one that every human has trod before us and will ever after. Just stumbling blindly along a tiny hyphen…between the words birth … and death.

exhales

And when reduced to that level of crisp simplicity…

Fear cannot exist.

Format of this thesis

The format of the thesis is in accordance with academic rule 5.4.2.7 stating: "Where a candidate is permitted to submit a thesis in the form of a published research article or articles or as an unpublished manuscript or manuscripts in article format and more than one such article or manuscript is used, the thesis must still be presented as a unit, supplemented with an inclusive problem statement, a focused literature analysis and integration and with a synoptic conclusion, and the guidelines of the journal concerned must also be included."

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STATEMENTS OF CO-AUTHORS

Contributions from the following co-authors are recognised, and their statements follow:

Prof. C.G. du Toit (page iv)

Dr. P.F. Niemand (page v)

Mr G.J. Nel (page vi)

Statement of consent: Prof. C.G. du Toit

To whom it may concern,

I, Charl Gabriel du Toit, give my consent to Ockert Cornelius Koekemoer, candidate for the degree Philosophiae Doctor in Nuclear Engineering at the North-West University, to include in his thesis entitled**: Investigation into different 1D/3D thermal fluid co-simulation methodologies as applied to HTR system configurations**, the following publications, of which I am a co-author:

Koekemoer, O.C., Nel, G.J. & Du Toit, C.G., 2019. ***Coupled 3D and 1D models of the heat transfer in a prismatic block of a VHTR.*** **Wicklow, Ireland, in: Proceedings of the 14th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics.**

Koekemoer, O.C., Du Toit, C.G, & Niemand P.F., 2021, Investigation into different 1D/3D co-simulation methodologies applied to a natural circulation loop, ***Nuclear Engineering and Design*****, Manuscript submitted for review/publication.**

Koekemoer, O.C. & Du Toit, C.G., 2021. Simulating heat transfer in a prismatic block VHTR using a 1D/3D thermal fluid co-simulation methodology, ***Nuclear Engineering and Design*** **Manuscript ready to be submitted for review/publication.**

Nel, G.J., Koekemoer, O.C. & Du Toit, C.G., 2019. ***1D and 3D CFD models of the heat transfer in a prismatic block of a VHTR.*** **Wicklow, Ireland, in: Proceedings of the 14th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics.**

The relative contributions to the paper by the different authors are given in each respective article. This statement serves to comply with academic rules 5.4.2.8 and 5.4.2.9 of the North-West University.

Signed at Potchefstroom on **25/11/2021**

Prof. C.G. du Toit

Statement of consent: Dr. P.F. Niemand

To whom it may concern,

I, Peter Franke Niemand, give my consent to Ockert Cornelius Koekemoer, candidate for the degree Philosophiae Doctor in Nuclear Engineering at the North-West University, to include in his thesis entitled: **Investigation into different 1D/3D thermal fluid co-simulation methodologies as applied to HTR system configurations**, the following publication, of which I am a co-author:

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Signed at Potchefstroom on **25/11/2021**

Dr. P.F. Niemand

Statement of consent: Mr G.J. Nel

To whom it may concern,

I, Gert Johannes Nel, give my consent to Ockert Cornelius Koekemoer, candidate for the degree Philosophiae Doctor in Nuclear Engineering at the North-West University, to include in his thesis entitled: **Investigation into different 1D/3D thermal fluid co-simulation methodologies as applied to HTR system configurations,** the following publications, of which I am a co-author:

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Co-authored Published Article (refer to **Annexure)**

Nel, G.J., Koekemoer, O.C. & Du Toit, C.G., 2019. *1D and 3D CFD models of the heat transfer in a prismatic block of a VHTR.* Wicklow, Ireland, in: Proceedings of the 14th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics.

The relative contributions to the paper by the different authors are given in each respective article. This statement serves to comply with academic rules 5.4.2.8 and 5.4.2.9 of the North-West University.

Signed at Potchefstroom on **25/11/2021**

Mr G.J. Nel

LIST OF PUBLICATIONS

The publications presented in this thesis in accordance with rule 5.4.2.8, are:

Koekemoer, O.C., Nel, G.J. & Du Toit, C.G., 2019. ***Coupled 3D and 1D models of the heat transfer in a prismatic block of a VHTR.*** **Wicklow, Ireland, in : Proceedings of the 14th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics.**

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To my big brother…
I am incredibly proud and in awe of all you have done and the remarkable person you are. You truly serve as one of my biggest inspirations and I truly hope that one day, you can be as proud of me as I am of you.
A special thanks to you.

SOLI DEO GLORIA

ABSTRACT

The current PhD research focuses on the investigation into different 1D/3D thermal fluid co-simulation methodologies as applied to HTR system configurations. For the modelling and simulation of complex systems, 1D/3D co-simulation is a promising approach used to aid in reducing the computational expense of the system under investigation. The required computational resources are optimized while maintaining an acceptable level of accuracy, by combining the desired features of a one-dimensional (1D) systems code with a three-dimensional (3D) Computational Fluid Dynamics (CFD) code.
Within this study the development and validation of different co-simulation strategies that couple the 3D CFD code, Ansys Fluent with the thermal-hydraulic systems code, Flownex were investigated.

To analyse radiative and convective heat transport as well as the natural circulation phenomena in a Reactor Cavity Cooling System facility, four different 1D/3D co-simulation methodologies were investigated. The 1D systems code, Flownex, and the 3D CFD code Ansys Fluent were used to perform the different 1D/3D co-simulations. Each code modelled a relevant part of the Reactor Cavity Cooling System (RCCS) facility and the models were coupled by explicitly exchanging boundary conditions or relevant data between the 1D and 3D regions. The corresponding temperatures, mass flow rates, and riser power of all four 1D/3D co-simulation approaches were found to be in good agreement with the results obtained from the validated full 1D simulation. The *directly coupled- parallel* model is the preferred strategy/approach as it requires less computational resources and reaches a converged solution in the least number of iterations and amount of solution time. Within the *directly coupled- parallel* approach, Ansys Fluent (3D code) provides the 1D code (Flownex) with the heat flux/heat transfer rate at the inside of the riser tubes, whilst the 1D code provides the 3D code with the temperatures of the inside surfaces of the riser tubes.

Using the *directly coupled-parallel* 1D/3D CFD approach (transferring surface temperatures and heat flux/heat transfer rates between the different codes/solvers) the heat transfer and fluid flow within a single-channel fuel module of a prismatic block VHTR was simulated. Validation of the coupled 1D/3D methodology was done using corresponding values obtained from published work and full explicit 3D CFD. When compared to an explicit 3D CFD analysis of the same system, the coupled 1D/3D projections suggest errors between the calculated fuel- and coolant temperatures of less than 1.5% for both a (i) uniform, and (ii) cosine power profile. When compared to explicit 3D CFD, the computational expense is greatly reduced by explicitly coupling the 1D and 3D solvers, whilst still retaining an acceptable level of accuracy. As a result, the 1D/3D co-simulation methodologies investigated within this study may be implemented for the thermal-hydraulic analysis of HTRs and accompanying systems.

*(**Keywords:** one dimensional, 1D, three-dimensional, 3D, coupled 1D/3D modelling, Computational Fluid Dynamics, numerical modelling, High Temperature Reactor, HTR, heat transfer)*

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1. INTRODUCTION

1.1 Background

Simulation-based assessments are frequently used in industry and academia to analyse a system's feasibility and performance. Due to the rising complexity of these systems, evaluating the overall behaviour at any stage of their implementation or development is becoming increasingly difficult. New techniques to efficiently simulate the interactions between subsystems are necessary to continue benefiting from the outcomes of the simulation-based analysis. There are two methods for accomplishing this: (i) monolithic simulation, in which the entire system/subsystem is represented and simulated using a single computational tool; or (ii) co-simulation, in which established computational tools for the various subsystems are coupled (Schwieger *et al*, 2019).

Simulation tools get increasingly specialized as our understanding of each subsystem grows, accumulating years of research and practical experience in their respective disciplines. As such, the use of the co-simulation approach allows existing simulation tools to be leveraged. Co-simulation has the ability to provide a fast and accurate technique to create holistic simulations by depicting interactions between subsystems and employing the best simulator/solver for each system. As a result, there has been an increase in the number of applications of co-simulation in a variety of fields (Aumiller *et al*., 2001, Galindo *et al*., 2011, Gonzalez-Albuixech e*t al*., 2016, Wang *et al*. 2017).

According to Hanna *et al*., (2017) and Schwieger *et al*. (2019) one-dimensional (1D) or three-dimensional (3D) Computational Fluid Dynamics (CFD) software is typically employed, when simulating and evaluating thermo-fluid systems.

Computational Fluid Dynamics (CFD) has long been utilized in a variety of industries, including aerospace, automotive, biomedical, chemical, marine, oil, gas, petrochemical, and power generation (Soumoy, 2010; Soumoy, 2019). Engineers can use one-dimensional (1D) CFD to see how flow rates and pressures fluctuate within a network of interconnected components. Three-dimensional (3D) CFD, on the other hand, allows designers and engineers to see how complicated geometry interacts with detailed flows (Linfield & Mudry, 2008). One-dimensional (1D) computations are substantially faster, taking only a few minutes versus hours or days for explicit 3D CFD. By coupling 1D and 3D CFD, the desired features of a one-dimensional (1D) systems code and a three-dimensional (3D) Computational Fluid Dynamics (CFD) code can be leveraged to help reduce the CFD computational expense whilst still retaining an acceptable level of accuracy.

1D/3D co-simulation includes several different possible implementations within the CFD industry. The focus of this study will be on 1D/3D fluid flow, mass-, and heat transfer systems. Hanna, *et al*., (2017) state that when coupling 1D and 3D CFD computational tools the following options exist:

- *3D CFD generated data inside a 1D CFD code*: The ability to loosely couple codes and enhance 1D CFD component libraries such as heat exchangers/pumps/turbines, etc. with performance data acquired from full 3D CFD component simulations exists within a 1D systems code.
- *Embedded Pseudo 3D CFD in a 1D CFD code:* A technique used to capture some three-dimensional effects within a one-dimensional systems code. For example, Simcenter's Flomaster software uses this technique to capture the effects of blockages between heat exchangers in automotive cooling packs (Mentor Graphics White Paper, 2017).
- *1D CFD elements embedded within 3D CFD codes:* The majority of multi-discipline CFD codes have 1D and 2D features. This allows for large physical domains to be modelled partially with large mesh cells and in other areas, that require little detail, to be dealt with in a computationally efficient 1D or 2D manner (Ansys, 2017 & CD-adapco, 2015).
- *General multi-dimensional 1D-2D-3D monolithic CFD:* A technique used where certain areas/parts of the flow domain are simplified to 2D or 1D and coupled with 3D predictions to help produce fast, relative accurate representations of complex systems.
- *1D/3D co-simulation CFD:* Different codes, each simulating a relevant part of the model are coupled by explicitly exchanging boundary conditions or relevant data between the 1D and 3D regions.

Most published articles consider the prevalent method of integrating 1D and 3D CFD (Aumiller, *et al*., 2001; Bavière, *et al*., 2014; Bertolotto, *et al*., 2009; Park, *et al*., 2013; Zhou, *et al*., 2017) to be 1D/3D co-simulation CFD. CFD boundary conditions from one solver update the boundary conditions of the second coupled solver, which then feed back to the original solver in the 1D/3D co-simulation. The data transfer between the different codes is performed iteratively until convergence is achieved.

1.2 Problem Statement

Co-simulation has been applied in various domains and scenarios, often without a comprehensive study on the impact to simulation- stability, time, and results. The goal of this research is to investigate different 1D/3D co-simulation strategies in the context of High Temperature Reactors (HTRs) and subsystems. The development and validation of different co-simulation strategies that couples the 3D CFD code, Ansys

Fluent (Ansys, 2017) with the thermal-hydraulic systems code, Flownex (M-Tech Industrial, 2019b) should be investigated.

1.3 Methodology

Using several coupling methodologies, a comprehensive study on the impact to simulation- stability, -time and results will be done on selected applications and subsystems within HTR systems, in order to test the validity of the coupled 1D/3D approach.

This study opted to investigate different 1D/3D co-simulation CFD methodologies available, by applying them to the simulation of the natural circulation occurring in a simplified Reactor Cavity Cooling System (RCCS). To analyse radiative and convective heat transport as well as the natural circulation phenomena in a Reactor Cavity Cooling System facility, four different 1D/3D co-simulation methodologies were investigated. The strategies included:

- (i) *directly coupled inline (domain decomposition)* model, where the entire test section (heater box) was modelled in 3D, and the remainder of the system was modelled using a 1D approach.
- (ii) *indirectly coupled parallel* model, where the outside wall of the heater box, air-cavity/cavities in the heater box, and the wall of the riser tubes in the heater box are modelled using the 3D approach. A 1D approach was employed to model the fluid flow in the pipe network, risers and the remainder of the system.
- (iii) *indirectly coupled parallel (domain overlapping*) model, which is similar to the first approach as the entire test section is modelled in 3D. However, the fluid flow in the pipe network, risers and the remainder of the system is modelled in 1D.
- (iv) *indirectly coupled parallel (flow resistive component)* model. Again, the entire test section is modelled in 3D. The remainder of the system is modelled in the 1D model as in the other models, whilst the flow in the risers is modelled using a flow resistance component which uses a representative resistance to determine the pressure drop over the test section

The 1D systems code, Flownex, and the 3D CFD code Ansys Fluent were used to perform the four different 1D/3D co-simulations. Each code modelled a relevant part of the Reactor Cavity Cooling System (RCCS) facility and the models were coupled by explicitly exchanging boundary conditions or relevant data between the 1D and 3D regions.

The behaviour and validity of the coupled 1D/3D approaches were investigated by comparing them with the full one-dimensional (1D) simulation of the simplified RCCS facility. The validity of the full 1D reference simulation was established by comparing the results predicted by the 1D simulation with the generalised correlation for steady-state turbulent flow in single-phase natural circulation loops.

The preferred 1D/3D co-simulation CFD methodology (*indirectly coupled parallel)* was subsequently employed to simulate the heat transfer and fluid flow within a single-channel fuel module of a prismatic block VHTR. Again, the one-dimensional (1D) systems code, Flownex, and the three-dimensional (3D) CFD code Ansys Fluent were used to perform the coupled 1D/3D simulations. Within the coupled 1D/3D models, the 1D elements represent the flow within the coolant channels while the spatial elements represent the fuel-compact and graphite moderator associated with the single-channel fuel module. Using the CFD code STAR-CCM+, a full 3D model consisting of the fuel compact, graphite moderator, and coolant channel of 1/6th of the SCFM was generated to validate the coupled 1D/3D model used within this study. This explicit 3D model was constructed to replicate the results obtained by Travis and El-Genk (2013b) and aid in the validation of the coupled 1D/3D methodology.

1.4 Contributions of the study

The following contributions are made in the current study:

- Coupled 1D and 3D models, used to simulate the heat transfer and fluid flow within a single-channel fuel module for a (i) uniform- and (ii) cosine power profile.
- Replicated a 3D explicit STAR-CCM+ model consisting of the fuel compact, graphite moderator and coolant channel of 1/6th of the SCFM to aid in the validity of the coupled 1D/3D models.
- Identified the shortcomings when using a coupled 1D/3D approach to simulate the heat transfer in a prismatic block VHTR.
    - The 1D/3D coupling strategy resulted in a stepwise constant profile for the axial variation in boundary values to be employed by Ansys Fluent.
    - Similarly, this stepwise profile was also reflected in the values obtained by the 1D/3D model for the variation in the temperature along the centreline of the fuel compact.
- Conducted a literature review on available options that exist when coupling 1D and 3D CFD computational tools as well as the different co-simulation strategies that exist when simulating an RCCS system which includes the Reactor Pressure Vessel (RPV) wall and cavity of the heater box, the risers, the inlet network and reservoir with the associated heat removal system.
- Four different 1D/3D co-simulation models employing Flownex and Ansys Fluent were created to investigate the radiative- and convective- heat transfer as well as the natural circulation phenomena occurring in a RCCS facility.
- A full one-dimensional reference simulation was constructed to investigate the behaviour and validity of the four 1D/3D coupled approaches.

- Applied the preferred **(updated)** 1D/3D co-simulation approach to the simulation of the heat transfer and fluid flow within a single-channel fuel module of a prismatic block VHTR.
  - Addressed the shortcomings identified and applied a smoother profile for the coolant wall temperatures used as boundary conditions in Ansys Fluent.
  - The solution strategy was also altered to make use of the new functionality that exists in Flownex, which allows for direct coupling with Ansys Fluent.

1.5 Thesis layout

Following the introductory chapter, the thesis consists of three original articles and one co-authored article (refer to **Annexure**), each of which will be presented in a respective chapter.

Chapter 2 presents the investigative conference article in which a coupled 1D/3D CFD model is used to simulate the heat transfer and fluid flow in a single-channel fuel module (SCFM). This peer-reviewed article was published in the Proceedings of the 14th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics (HEFAT 2019).

Chapter 3 contains the second article. In the second article four different co-simulation approaches were explored to investigate the radiative- and convective- heat transfer, and natural circulation phenomena occurring in a simplified water-cooled RCCS facility. The impact on simulation- stability, -time, and results were investigated to help serve as a basis for future 1D/3D co-simulation implementations. This article was submitted to Nuclear Engineering and Design for review and possible publication in the international journal *Nuclear Engineering and Design*.

Chapter 4 consists of the third article, within this article the heat transfer in a prismatic block VHTR is simulated using a coupled 1D/3D methodology. It is worth noting that even though the same SCFM was simulated as in article 1 (Chapter 2), the solution strategy and the methodology used to transfer data is different. Also, within this article, the shortcomings identified within the first article were addressed. This article is ready to be submitted for review and possible publication in the international journal *Nuclear Engineering and Design*.

Chapter 5 provides a summary of the main conclusions of the three original articles (Chapter 2,3, and 4) as well as recommendations for future work.

Lastly, the Annexure contains a co-authored article that was also presented and accepted for publication in the HEFAT 2019 proceedings.

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2. ARTICLE 1: COUPLED 3D AND 1D MODELS OF THE HEAT TRANSFER IN A PRISMATIC BLOCK OF A VHTR

O.C. Koekemoer*, G.J. Nel and C. G. du Toit

Abstract:

Modelling prismatic block high-temperature gas-cooled reactor units pose several challenges and typically requires significant computational resources and computational times. This is largely due to the complexity of prismatic block reactor models as these models must amongst others account for the fuel-compacts, graphite, and coolant channels in fuel blocks, cross- and bypass gaps between blocks and the mixing in the lower plenum. This amount of detail however cannot be dealt with in a single explicit three-dimensional model.

Motivated by recent advances in the field of Computational Fluid Dynamics (CFD) and recognizing the limitations on available computing power, this article is aimed at combining the desired features of a one-dimensional (1D) system code and three-dimensional (3D) CFD code. The goal is achieved by demonstrating the coupled 3D/1D CFD model that simulates the heat transfer and fluid flow in a single-channel fuel module of a prismatic block. The coupled 3D/1D model represents one-sixth of a single-channel fuel model that accounts for conduction heat transfer in the solids (fuel compact and graphite moderator), convection heat transfer between the solids and the fluid (helium) and the fluid flow in the coolant channel. The validity of the coupled 3D/1D model is investigated by comparing the temperature distribution in the single-channel fuel model for a (i) uniform- and (ii) cosine power profile with the corresponding values obtained from published work as well as a full detailed 3D CFD analysis of the same specifications and setup. Since the 3D/1D models require significantly less resources than the detailed 3D CFD it can form the basis of an integrated model for the entire core.

Keywords:

1D/3D co-simulation, CFD, heat transfer, VHTR. Single-channel fuel Module (SCFM)

1. Introduction

The Very High Temperature Reactor (VHTR) is a graphite-moderated helium-cooled reactor capable of delivering thermal power of up to 600 MW_{th}. A potential benefit of the VHTR is that reactor outlet temperatures of as high as 1000 °C may be achieved for process heat and hydrogen production applications. However, the main focus at present is on the lower outlet temperatures as industrial processes and electricity production based on steam in the range of 700-850 °C already have great potential and present significantly less technical risks (GIF, 2014). The VHTR's inherent safety, high thermal efficiency and high-temperature process heat led to the development and implementation of generation–IV, prismatic core, VHTRs. These reactors require demonstrable and effective computational tools and methodologies for the design, operation, and safety analyses (Schultz, *et al*., 2004).

In a prismatic VHTR, TRISO (Tristructural-isotropic) particles are bonded together with a carbonaceous matrix into rod-shaped fuel compacts, which are stacked in the fuel holes of hexagonal graphite blocks. One of the challenging design issues in the development of the VHTR is an undesirably high temperature of the nuclear fuels in prismatic cores. Such a high fuel temperature affects the integrity of the TRISO particles as well as the fission products released (Tak, *et al*., 2008). A high fuel temperature is therefore directly related to the increased core outlet temperature of the VHTR. To satisfy the widely accepted design limit (~1250 °C) the maximum temperature difference between the fuel and the coolant should be less than ~250 °C (Collins, 2009; IAEA, 1990). Considering the low heat transfer characteristics of the coolant (i.e., helium) and the non-uniform power distribution in the reactor core, the fuel temperature limit is a critical issue for the design of the VHTR. An understanding of the thermal behaviour of the prismatic fuels and the capability for an accurate prediction of the fuel- and coolant temperatures are therefore of considerable importance in the design of VHTRs. However, the complex geometry and nature of the numerical models hinders accurate evaluations of the fuel- and coolant temperatures without extensive numerical calculations.

Nuclear system codes such as Relap5 (INL, 2018), TRAC (Jenkins *et al*., 1988), CATHARE (IRSN, 2006) and Flownex (M-Tech Industrial, 2019b) are widely used to investigate the thermal-hydraulic characteristics of the nuclear power plants (NPPs) either under normal steady-state conditions or during various accident scenarios. CFD codes such as STAR-CCM+ (CD-adapco, 2015), CFX (Ansys, 2017) and Fluent (Ansys, 2017) are also widely employed in nuclear reactor safety and design to analyse important and noticeable 3D effects. By combining 3D CFD codes and system codes, the advantageous coupled 3D/1D CFD approach can form the basis of an integrated model of the entire core. Explicit or semi-implicit coupling methodologies are available when coupling 3D CFD and systems CFD codes. Explicit methodology requires that the data are exchanged between the codes only once for each time-step. However, for the semi-implicit methodology, the data are exchanged several times for each time-step until convergence of the coupled parameters is reached.

This paper demonstrates a 3D/1D approach that couples Ansys Fluent and Flownex in an explicit manner by simulating the heat transfer and fluid flow in a single-channel fuel module.

2. Single-channel fuel module

The inner core section of a prismatic VHTR consists of columns of fuel assemblies with graphite reflector blocks at the top and bottom ends of the fuel assemblies. The graphite reflectors are added to reduce the amount of neutron leakage out of the system. A typical fuel block consists of 210 holes for the rod-shaped fuel compacts and 102 coolant holes. Ten fuel blocks, each with a height of 800 mm, are stacked to form a fuel block assembly which has a total length of 8000 mm (Travis & El-Genk, 2013b).

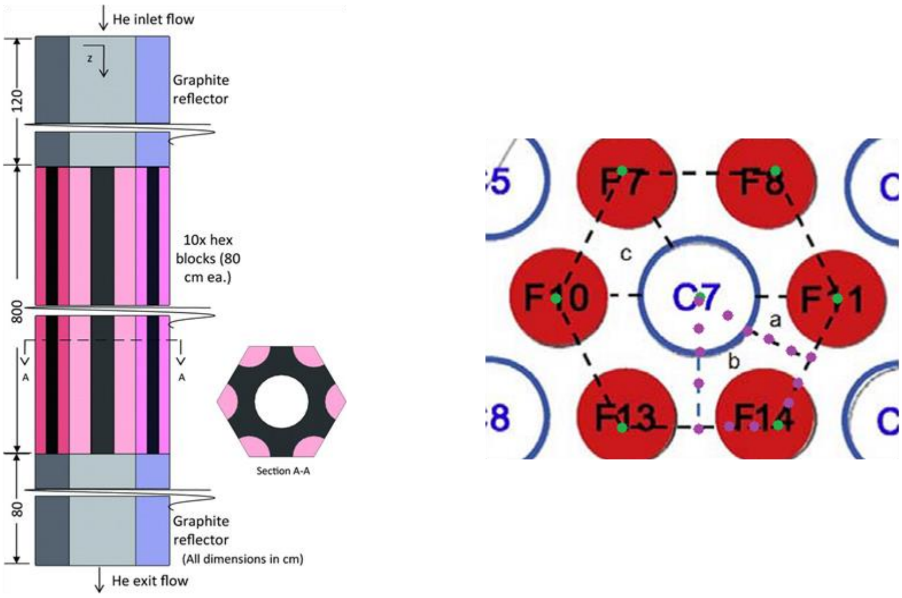
A Single-Channel Fuel Module (SCFM) of a prismatic core block is shown in Fig. 1(a) and Fig. 1(b), where the red elements in Fig. 1(b) represent the fuel compacts and the blue elements represent the coolant channels. A pattern of one single coolant channel surrounded by six fuel channels is repeated throughout the hexagonal blocks in the core. The SCFM is represented by the hexagonal cross-section contained around the coolant channel in Fig. 1(a) and the area outlined by the dashed hexagon in Fig. 1(b). The fuel compacts have a diameter of 12.7 mm whereas the diameter of the coolant channels is 15.875 mm. The fuel compact pitch is 37.6 mm.

Based on the symmetry that can be observed in Fig. 1(b) only a section of the SCFM needs to be modelled. Fig. 1(b) illustrates three-unit cells, indicated by the dashed areas *a*, *b*, and *c*. Unit cell *a* represents 1/12th of the SCFM, whilst unit cells *b* and *c* represent 1/6th of the SCFM. Unit cell *b* was selected for this study as Sambureni (2015) had already characterized the conduction shape factors for this unit cell.

As boundary conditions for the SCFM an inlet- temperature and pressure of 914 K and 7.07 MPa respectively was assumed, with a mass flow rate of 0.0306 kg/s for the coolant. A power of 55.4 kW was applied to the SCFM, which corresponds to 600 MW_{th}. Two power profiles were assumed, a (i) uniform- and (ii) cosine power distribution. In the case of the uniform distribution a power density of 27.406 MW_{th}/m^3 was prescribed (Travis & El-Genk, 2013b). For the cosine power profile, the power density $PD(z)$ at a distance z from the entrance of the coolant channel is given as:

$$PD(z) = PD_{max}\cos(0.2566z - 0.8831) \quad (1)$$

With a maximum power density of $PD_{max} = 33.135$ MW_{th}/m^3.



(a) (b)

Figure 1: (a) Side and top view of the SCFM (Travis & El-Genk, 2013b)**; and (b) dashed hexagon outlining SCFM cross-sectional area** (Sambureni ,2015).

The properties of the different materials are summarized in Table 1.

Table 1: Material properties used in SCFM (Travis & El-Genk, 2013b).

Property	Material	Correlation
Density, ρ (kg/m^3)	IG-110 graphite	1740
Specific heat, C_p (J/kg.K)		$6.05*10^{-7}T^3$ -0.00269T^2 +4.19T -294
Thermal conductivity, k (W/m.K)		-13.2 +2.50*10^4/$(T+268)^{0.78}$
Density, ρ (kg/m^3)	Composite Fuel	1650
Specific heat, C_p (J/kg.K)		$3.11*10^{-7}$ T^3 -0.00155 T^2 +2.73 T -82.4
Thermal conductivity, k (W/m.K)		8.5 +7.68*10^4/$(T+268)^{0.995}$
Density, ρ (kg/m^3)	Helium	P/R_gT
Specific heat, C_p (J/kg.K)		5197.6
Thermal conductivity, k (W/m.K)		0.000258 T +0.103388
Dynamic viscosity, µ (Pa-s)		0.03319 T +13.0744

3. Single-channel fuel module modelling

Coupling explicit 3D- and 1D models require that appropriate convection heat transfer correlations be used. Travis & El-Genk (2013b) performed an explicit 3D detailed simulation of a single-channel fuel module (SCFM) using the CFD code STAR-CCM+, to evaluate various convection heat transfer correlations. Based on the results obtained by Travis & El-Genk (2013a) it was found that the convection heat transfer regime can be considered as turbulent forced convection heat transfer. They then proposed an improved convection heat transfer correlation and implemented that in a coupled 3D/1D simulation of the SCFM. STAR-CCM+ was used to model the 3D heat transfer. However, no information is given on the 1D formulation that Travis & El-Genk employed. A 1D model of the fuel compact, graphite moderator and coolant channel using the systems code Flownex was constructed by Nel & Du Toit (2018). They implemented the convection heat transfer coefficient correlation proposed by Travis & El-Genk (2013b) and found the coolant wall temperatures to be in good agreement with the corresponding temperatures obtained by Travis & El-Genk (2013a).

In this study, models were considered that represent 1/6th of the cross-section of the SCFM considered by Travis and El-Genk (2013b). The results obtained from the coupled 3D/1D method are compared to the values published by Travis & El-Genk (2013a, 2013b).

4. 3D STAR-CCM+ Model

An explicit 3D model of the fuel compacts, graphite moderator and coolant channel of 1/6th of the SCFM was created using the CFD code STAR-CCM+. This model was constructed to recreate the results that were obtained by Travis & El-Genk (2013b) as well as aid in the investigation of the validity of the coupled 3D/1D model. The geometry of the entire SCFM model was constructed in Solidworks (Dassault Systems, 2017) and consisted of a 1200 mm long section of the 1/6th SCFM. The assembly was imported into STAR-CCM+ and the associated physics continua associated with the fuel compact, graphite moderator and coolant channel were assigned. The material properties listed in Table 1 were used in both the STAR-CCM+ and Ansys fluent models. A single mesh continuum was constructed for all the components in the STAR-CCM+ model to ensure that the cell faces on the interfaces between adjacent parts matched to form a conformal mesh. This ensured that no interpolation was necessary for the transfer of information across interfaces. It was found to play an important role in the stability of the solution. A basic base size of 6mm, based on the radius of the fuel compact, was chosen for the mesh. A total thickness for the five prism layers together was 0.4 mm with a layer stretched factor of 1.2. This ensured that the temperature gradients at the interfaces were resolved sufficiently and assisted in the stability of the solution.

The prism layers, mesh, and conformal mapping across the interfaces of the generated mesh that was set up in STAR-CCM+ can be seen in Fig. 2.

The mesh for the 1200 mm section of the SCFM was created. The mesh was then used as the basis for the extrusion meshing scheme used within the simulations.

The total length of the 1/6th SCFM was assumed as 9200 mm to account for the top reflector and the height of 8000 mm of the heated section as shown in Fig. 1(a).

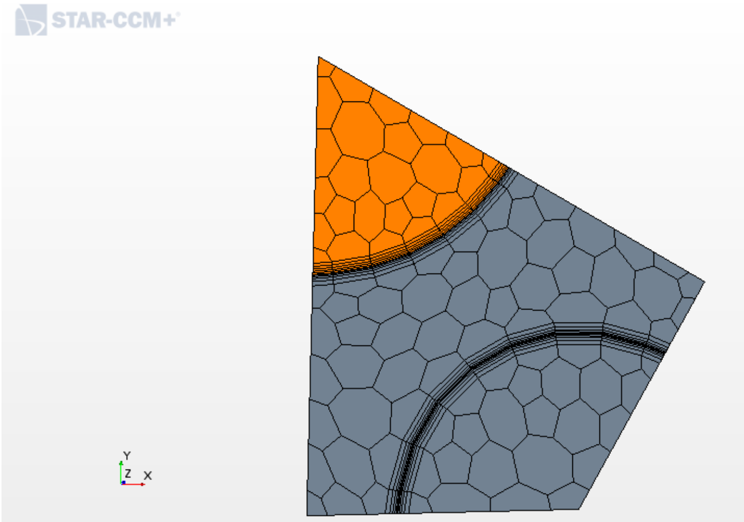


Figure 2: Cross-section of STAR-CCM+ mesh.

Travis & El-Genk (2013b) commented that the 1200 mm length of the reflector is 75 coolant channel diameters which is sufficient for fully developed turbulent flow to occur at the entrance to the heated section.

The extrusion mesh consisted of 11500 layers that resulted in a layer having a thickness of 0.8 mm, similar to that used by Travis & El-Genk (2013b). New interfaces between the fuel compact and graphite moderator and between the graphite moderator and coolant channel had been created. This was done to ensure a uniform mesh distribution within the axial direction.

5. 3D/1D Coupling Methodology

Similar to Travis & El-Genk (2013b) the SCFM was also modelled using a 3D CFD approach to simulate the heat transfer in the fuel compact and the graphite moderator and the 1D approach to simulate the fluid flow in the coolant channel. The coolant channel was modelled in Flownex while the fuel compact and the moderator were modelled in Ansys Fluent. During the simulation, the two codes transfer the relevant data between each other in an explicit manner.

5.1 3D Simulation procedure

As Flownex only accounts for the mass flow rate and the associated average velocity in the coolant channel, the coupled 3D/1D CFD model only considers the 8000 mm heated section of the SCFM, and the reflector block is therefore not needed for the velocity profile to develop. Similar to the 3D STAR-CCM+ model, the 3D geometry of the SCFM consisting of the fuel compact and graphite moderator was assembled in Solidworks and imported into Ansys Fluent. This model was then divided into forty-nine axial increments corresponding to the axial increments of the Flownex model described in the section below. The different increments of the fuel compact and the graphite moderator were categorized and assigned to reflect their nature, e.g., symmetry planes and walls. In the Ansys Fluent model, prism layers were only defined on the moderator side of the coolant channel wall. A sweep-and-assembly meshing scheme was adopted to ensure a conformal mesh throughout the entire model. The same meshing and solution strategies and material properties were applied as in the 3D STAR-CCM+ model. The conformal mapping across the interfaces and prism layers of the generated mesh can be seen in Fig. 3 and as well as the mesh that was set up in Ansys Fluent for the graphite moderator and fuel compact.

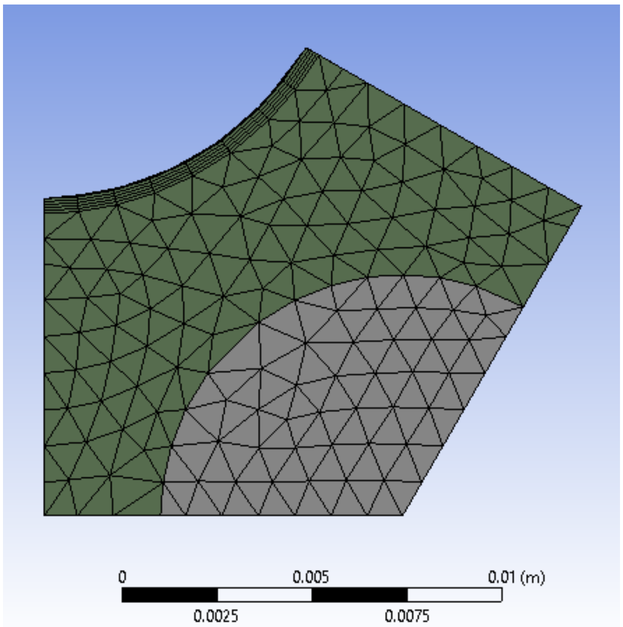


Figure 3: Cross-section through Ansys Fluent mesh.

After the mesh was completed, the input and output parameters (to be transferred between Flownex and Ansys Fluent) as well as the different boundary conditions were set up and assigned. The power profiles for (i) uniform- and (ii) cosine power distributions were applied as volumetric heat sources by using UDFs in Ansys Fluent.

5.2 1D Simulation procedure

The flow in the coolant channel was simulated in Flownex. Similar to the 3D Ansys Fluent model, the 1D model is divided into forty-nine axial increments. The first 10 increments are each 40 mm in length followed by two 100 mm increments and then thirty-seven increments each 200 mm in length. This model uses only the convection and pipe elements and their corresponding nodal elements to represent the flow and convection heat transfer in the coolant channel. The properties of the pipe and convection components were similar to those used in the full 1D Flownex simulation by Nel & Du Toit (2018).

The boundary conditions at the inlet and the outlet of the coolant channel were the same as the corresponding boundary conditions used by Nel & Du Toit (2018) for the full 1D Flownex simulation. The inlet and first increment of the Flownex model are shown in Fig. 4.

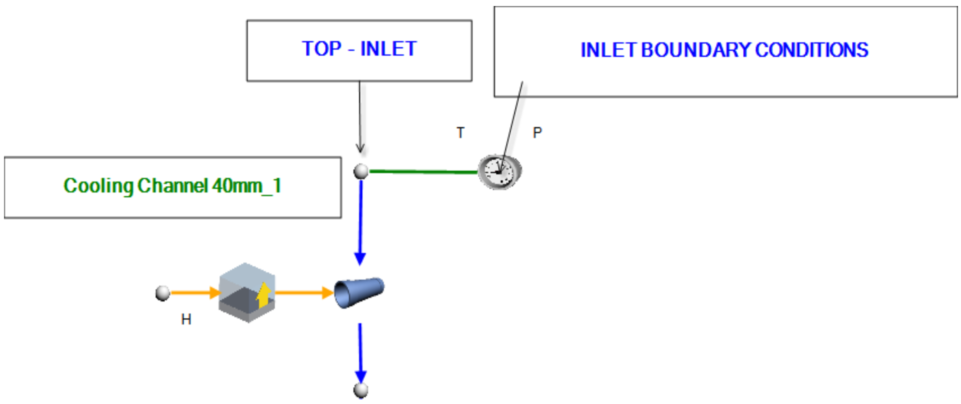


Figure 4: Inlet and first increment of the coupled Flownex model.

5.3 3D/1D coupling procedure

After the 3D Ansys Fluent model and the 1D Flownex model were constructed, the two codes had to be coupled to each other in order to define the data to be transferred between the two models. Flownex was chosen as the managing code and to run Ansys Fluent in server mode. In Flownex a Server Fluent Generic Interface component was inserted to control the transfer of data between Flownex and Ansys Fluent. In the Flownex model data transfer links that couple the Flownex wall nodes to the relevant Ansys Fluent input/output parameters to account for the exchange of the coolant channel wall temperatures and the heat released by the coolant channel wall is defined. In Fig. 5 a representation can be seen of the main coupled model in Flownex where the dashed lines signify the data transfer links to and from Ansys Fluent. Data transfer links must be defined for all the increments. Information transfer is initialized after steady-state solutions for both Flownex and Fluent are achieved. The coupled simulation could then be started. In Flownex the wall temperature is transferred to Ansys Fluent to the corresponding increments. In Ansys Fluent a heat transfer report is used to transfer information for the heat generated to the corresponding elements in Flownex.

After the coupling of the two codes, an iterative procedure was followed in which Flownex completed a number of iterations and then transfers the necessary data to Ansys Fluent. Ansys Fluent then initialized with the inputs received and completed a number of iterations before the necessary information was sent back to Flownex. This procedure was repeated until the specified convergence criteria were met.

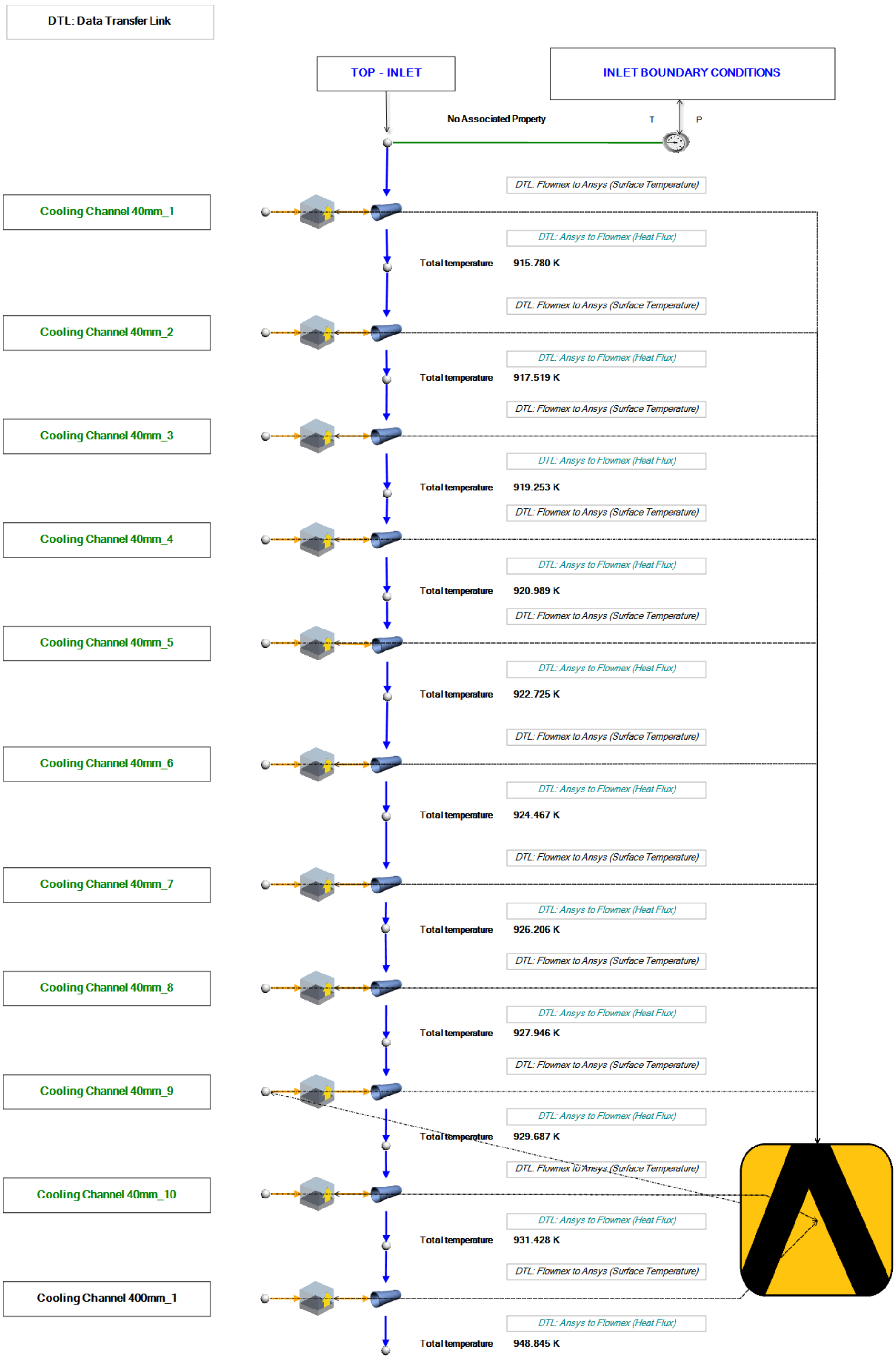


Figure 5: Flownex/Ansys Fluent coupling.

6. Numerical Results and Discussions

The validity of the coupled 3D/1D model is investigated by comparing the temperature distribution in a single-channel fuel module for a (i) uniform- and (ii) cosine power profile with the corresponding values obtained from a full 3D CFD analysis of the same specification and setup.

In Fig. 6 the axial variation in the temperature at the centre of the fuel compact for the uniform and cosine power profile as obtained in the 3D/1D model is compared with the corresponding results obtained in the full 3D STAR-CCM+ model. It can be seen that the agreement for both the uniform- and cosine power profiles is very good.

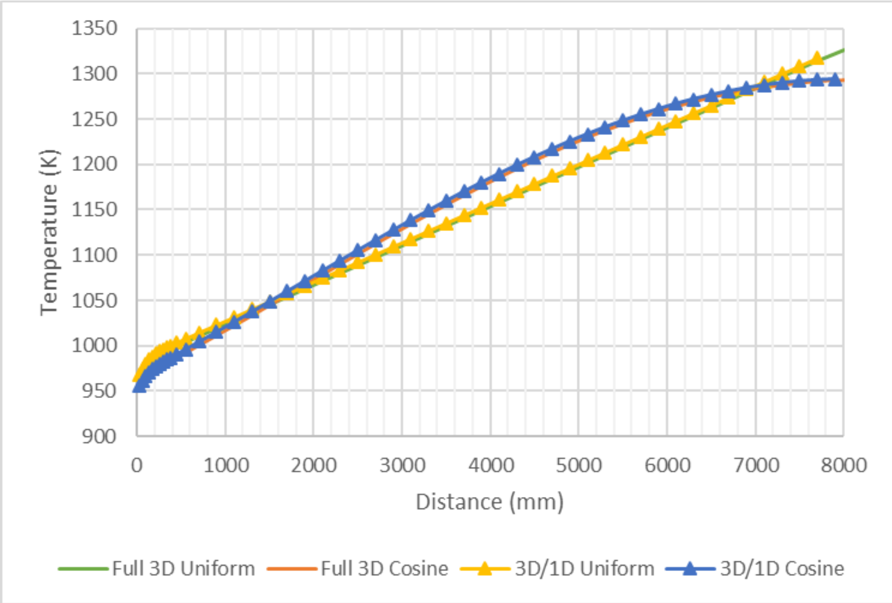


Figure 6: Fuel compact temperature as a function of axial position for the uniform and cosine power profiles.

Fig. 7 shows the comparison between the results obtained by the 3D model and the 3D/1D model for the variation in the axial direction of the coolant wall temperature for both the cosine- and uniform power profiles. It can again be seen that the agreement between the corresponding results is very good.

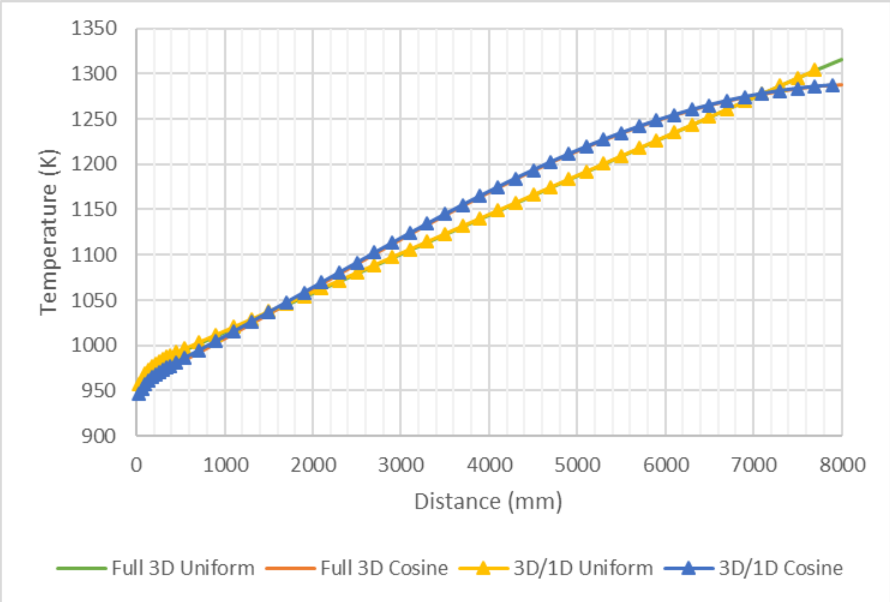


Figure 7: Coolant channel wall temperature as a function of axial position for the uniform and cosine power profiles.

The coolant wall temperatures provided by each Flownex increment in the coupled 3D/1D simulation to the corresponding Ansys Fluent coolant wall increments are received by Ansys Fluent as a constant value for each wall increment. This then results in a stepwise constant profile for the axial variation in the boundary values employed by Ansys Fluent for the coolant wall temperature. This is also reflected in the values obtained by the 3D/1D model for the variation in the temperatures along the centreline of the fuel compact. The temperature profiles shown in Fig. 7 are based on the temperatures that were extracted at the centre of each axial increment.

Fig. 8 and Fig. 9 show the radial temperature distributions at three different axial locations within the SCFM obtained by the full 3D model and by the coupled 3D/1D model. The radial distributions are from the centre of the coolant channel to the centre of the fuel compact. Fig. 8 shows the results for the uniform power profile, whilst Fig. 9 illustrates the results for the cosine power profile.

From Fig. 8 and Fig. 9, it is evident that the coupled 3D/1D model can only predict the bulk fluid temperature. Although not shown in the figures, it was found that the bulk temperatures of the fluid predicted by the coupled 3D/1D models were in very good agreement when compared to the full 3D STAR-CCM+ models with a maximum of 3% deviation between the models. The temperature variations for the fuel compact and the graphite moderator predicted by the coupled 3D/1D model and the full 3D model are also in very good agreement.

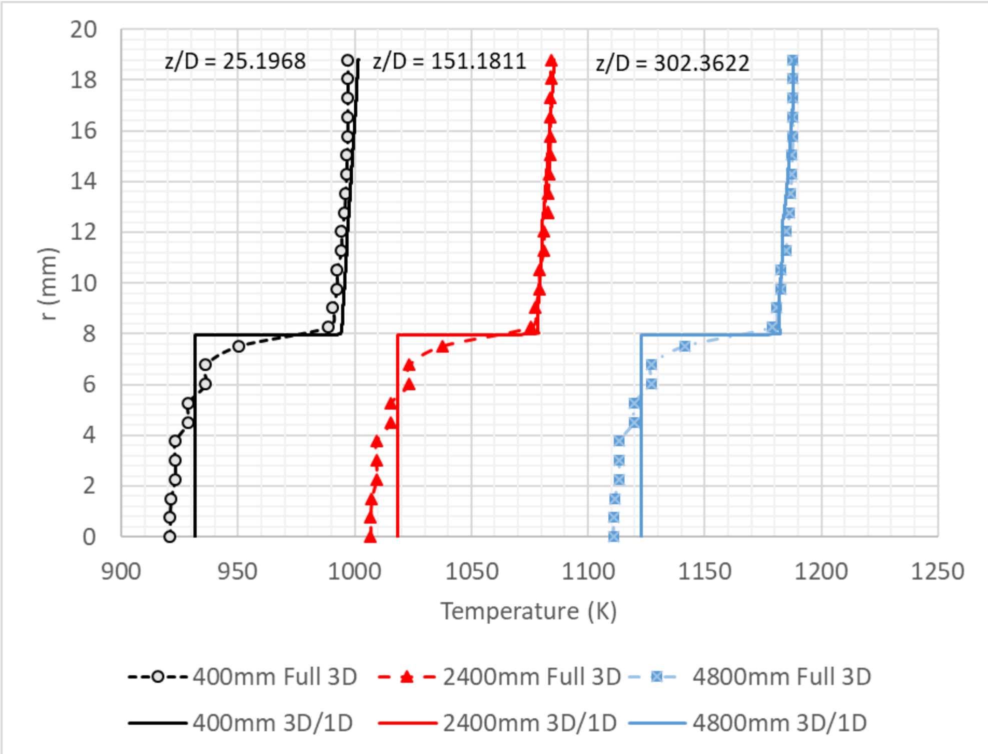


Figure 8: Radial temperature distribution at three axial locations for the 3D and 3D/1D uniform profile.

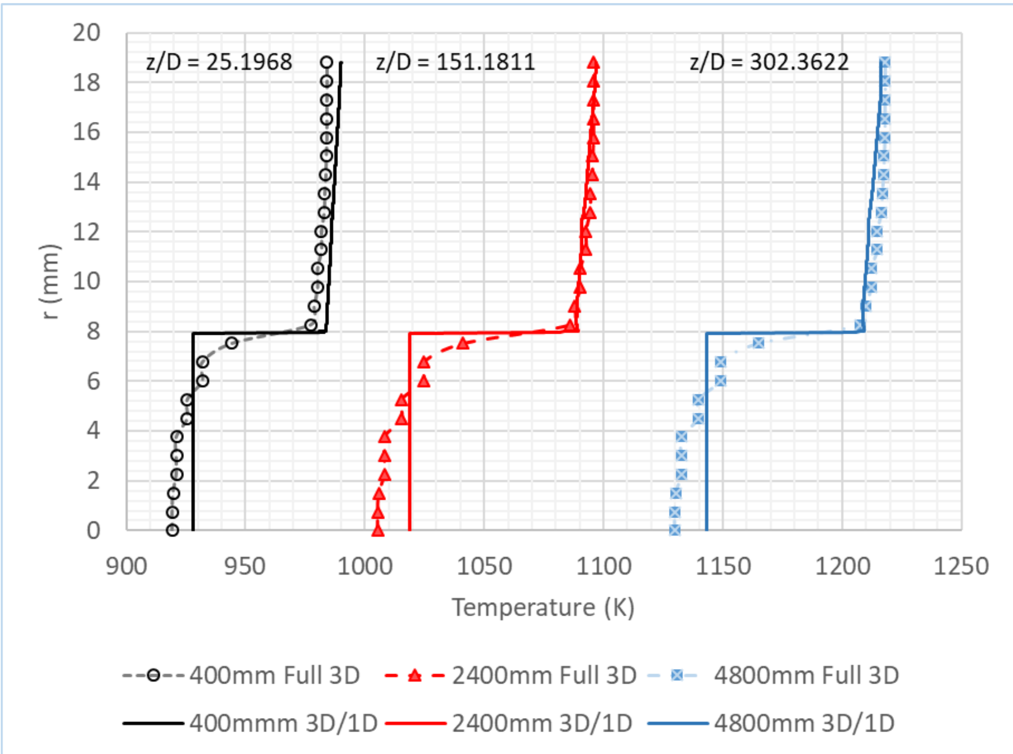


Figure 9: Radial temperature distribution at three axial locations for the 3D and 3D/1D cosine profile.

7. Summary and Conclusion

Understanding the thermal behaviour and predicting accurate fuel- and coolant temperatures are of considerable importance in the design of VHTRs. This paper discussed coupled 3D/1D CFD- and full 3D CFD models that simulate the heat transfer and fluid flow in a single-channel fuel module of a prismatic block. The study performed by Travis & El-Genk (2013b) on the numerically modelling of the heat transfer and flow in a SCFM was used as the basis for the current study.

The validity of the coupled 3D/1D model was investigated by comparing the temperature distribution in the single-channel fuel model for a (i) uniform- and (ii) cosine power profile with the corresponding values obtained from published work as well as a full detailed 3D CFD analysis of the same specifications and setup. The models developed in this study considered only 1/6th of the cross-section of the SCFM simulated by Travis & El-Genk (2013b) due to the symmetry in the geometry of the SCFM. An explicit 3D model of the fuel compact, graphite moderator and coolant channel of the 1/6th of the SCFM was created using the CFD code STAR CCM+. The coupled 3D/1D model of the 1/6th SCFM was generated using Ansys Fluent for the explicit 3D representation of the fuel compact and graphite moderator and the system CFD Flownex for the 1D representation of the coolant channel. The Travis & El-Genk convection heat transfer correlation was employed to couple the heat transfer between the 3D and 1D formulations. The results for the coolant channel wall temperatures and fuel compact centre temperatures were found to be in very good agreement with corresponding values predicted by the full 3D explicit model.

It can therefore be concluded that the coupled 3D/1D simulation provides results for the coolant wall and fuel compact temperatures that are in very good agreement with the coolant wall and fuel compact temperatures obtained by the full 3D simulation. Due to the marked reduction in the grid requirements for the modelling of the flow in the coolant channel in the coupled 3D/1D model compared to the full 3D model, it also leads to a reduction in the computational resources required. However, the coupling strategy used to transfer the relevant data between Ansys Fluent and Flownex should be investigated to determine whether it might be possible to transfer a smoother profile for the coolant wall temperatures to be used as boundary conditions in Ansys Fluent.

CRediT authorship contribution statement

O.C Koekemoer: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Writing – Original Draft, Project administration.

G.J. Nel: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation.

Prof. C.G. du Toit: Conceptualization, Supervision, Writing – review and editing. Project administration.

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Any opinion, finding and conclusion or recommendation expressed in this material is that of the author(s) and the NRF does not accept any liability in this regard.

Nomenclature

Abbreviations

1D	One-dimensional
3D	Three dimensional
CFD	Computation Fluid Dynamics
NPPs	Nuclear Power Plants
SCFM	Single-Channel Fuel Module
TRISO	Tristructural-isotropic
VHTR	Very High Temperature Reactor
UDF	User Defined Function

Symbols

c_p	[J/kg.K]	Specific heat
D	[m]	Diameter
k	[W/m.K]	Thermal conductivity
μ	[Pa-s]	Dynamic viscosity
ρ	[kg/m^3]	Density
T	[K]	Temperature
z	[m]	Cartesian axis direction

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3. ARTICLE 2: INVESTIGATION INTO DIFFERENT 1D/3D CO-SIMULATION METHODOLOGIES APPLIED TO A NATURAL CIRCULATION LOOP

O.C. Koekemoer*, C. G. du Toit and P.F. Niemand

Abstract:

1D/3D co-simulation is a promising approach for the modelling and simulation of complex systems. These systems are typically computationally intensive. By combining the desired features of a one-dimensional (1D) systems code and a three-dimensional (3D) Computational Fluid Dynamics (CFD) code, the required resources are optimized whilst still retaining an acceptable level of accuracy. Co-simulation has been applied in various domains and scenarios, often without a comprehensive study on the impact to simulation-stability, -time, and results. The purpose of this study is to explore the behaviour of some of the strategies by applying them to the simulation of the natural circulation occurring in a simplified Reactor Cavity Cooling System (RCCS). Four different co-simulation approaches were explored to investigate the radiative- and convective- heat transfer as well as the natural circulation phenomena occurring in a RCCS facility. Typically, in these four modelling approaches a 3D methodology was employed to model the radiation and convection heat transfer in the cavity between the heater wall and the outer wall of the riser. The 1D methodology was employed to model the remainder of the RCCS system. The 1D systems code, Flownex, and the 3D CFD code Ansys Fluent were used to perform the 1D/3D co-simulations. Each of the codes modelled a relevant part of the RCCS facility and the models were coupled by explicitly exchanging boundary conditions or relevant data between the 1D and 3D regions. The validity of the coupled 1D/3D approaches was investigated by comparing them with a full 1D simulation.

Keywords:

1D/3D co-simulation, CFD, heat transfer, RCCS, natural circulation.

1. Introduction

In various fields in industry and academia, design engineers and analysts use simulation-driven assessments to determine the performance characteristics and feasibility of a system. Primarily, 1D or 3D CFD software is used when simulating and evaluating thermo-fluid systems (Hanna, *et al.*, 2017; Schwieger & Gomes, 2019). Three-dimensional (3D) CFD can be extremely accurate when designing and simulating complex systems, as it can calculate much more detailed flow field predictions using more detailed physical models (Linfield & Mudry, 2008). However, simulating complex systems in detailed 3D CFD can be computationally expensive, as a single simulation can take several days/weeks to run depending on the size of the model being used and require extensive computational resources.

One dimensional (1D) CFD on the other hand, is a faster solution approach taking a fraction of the time to run but requires a significant amount of real-world test data to characterize the more complex 3D components of the system accurately (Hanna, *et al*., 2017). 1D CFD enables the hydrodynamic and thermal behaviour of a complex network of piping systems to be investigated. The computational efficiency of systems-level tools allows for complete descriptions of entire arrangements to be considered, without the need to impose uncertain localized boundary conditions, as in the case of 3D CFD. This is achieved by using thermo-fluid catalogues, of representative components such as pipes, valves, bends, reservoirs, pumps, heat exchangers, etc., hydrodynamically (M-Tech Industrial, 2019b; Hanna, *et al*., 2017; Soumoy, 2010).

To keep benefiting from simulation-based analyses, new techniques are required to efficiently simulate the interactions between subsystems. According to Schwieger & Gomes (2019), two possible techniques exist to achieve this end: (i) monolithic simulation, where the entire system is being simulated using a single 1D or 3D computational tool; or (ii) co-simulation, where established computational tools are coupled for the respective subsystems.

1D/3D co-simulation includes several different possible implementations within the CFD industry. In the context of this paper, the focus will be on 1D/3D fluid flow, mass-, and heat transfer systems. As a result, Hanna, *et al*., (2017) note that the following options exist when coupling 1D and 3D CFD computational tools.

- *3D CFD into a 1D CFD code*: The ability exists within a 1D systems code to loosely couple codes and extends 1D CFD component libraries such as heat exchangers/pumps/turbines etc. with performance data gathered from full 3D CFD component simulations.

- *Embedded Pseudo 3D CFD in a 1D CFD code:* A technique used to capture some three-dimensional effects within a 1D systems code. For example, Simcenter's Flomaster software uses this technique to capture the effects of blockages between heat exchangers in automotive cooling packs (Mentor Graphics White Paper, 2017).

- *1D CFD elements embedded within 3D CFD codes:* Most multi-discipline CFD codes have some kind of 1D and 2D elements embedded within. This allows for large physical domains to be modelled partially with large mesh cells and in other areas, that require little detail, to be dealt with in a computationally efficient 1D or 2D manner (Ansys, 2017; CD-adapco, 2015).

- *General multi-dimensional 1D-2D-3D monolithic CFD:* A technique used where certain areas/parts of the flow domain are simplified to 2D or 1D and coupled with 3D predictions to help produce fast, relative accurate representations of complex systems.

- *1D/3D co-simulation CFD:* Different codes, each simulates a relevant part of the model are coupled by explicitly exchanging boundary conditions or relevant data between the 1D and 3D regions.

The dominant method of integrating 1D and 3D CFD is considered in most published papers (Aumiller, *et al*., 2001; Bavière, *et al*., 2014; Bertolotto, *et al*., 2009; Park, *et al*., 2013; Zhou, *et al*., 2017) to be 1D/3D co-simulation CFD. Within 1D/3D co-simulation CFD boundary conditions from one solver update the boundary conditions of the coupled-solver, which in turn feedback to the original solver. This iterative process of data transfer between the different codes is repeated until convergence is achieved.

In 1D/3D co-simulation, the desired features of a one-dimensional (1D) systems code and a three-dimensional (3D) Computational Fluid Dynamics (CFD) code can be leveraged to help reduce the CFD computational expense whilst still retaining an acceptable level of accuracy. This study opted to investigate different 1D/3D co-simulation CFD strategies available, by applying them to the simulation of the natural circulation occurring in a simplified Reactor Cavity Cooling System (RCCS).

In a study conducted by Zhou, *et al*., (2017), a 1D/3D coupling methodology was developed to investigate the flow characteristics of a pump system during start-up conditions of the Passive Residual Heat Removal System (PRHRS). The coupled 1D/3D methodology used Flowmaster to simulate the pipe network while the flow characteristics within the pump were simulated using CFX. During the co-simulation a third code, MpCCI was introduced to transfer data between the codes on the interface. Inlet pressure and outlet mass flow rate were transferred to the 3D domain. In the 1D domain, the inlet pressure and mass source were specified for the domain boundary (Zhou, *et al*., 2017). Data transfer occurred iteratively for each timestep until convergence occurred.

Zhao, *et al*., (2019) used a coupled model to analyze the transient characteristics of the Passive Residual Heat Removal System (PRHRS) of the HTR-10. Within the study Zhao, *et al*., (2019) used a one-dimensional code developed using the C programming language to simulate the pipe network before and after the cavity. Ansys Fluent was implemented to model the Cavity in a three-dimensional manner. Similar coupling methodologies of a computational fluid dynamics code and a system code can be found in the open literature (Aumiller, *et al*., 2001; Bavière, *et al*., 2014; Bertolotto, *et al*., 2009).

Kööp (2018) simulated the TALL test facility, by coupling the thermal-hydraulic systems code RELAP and the computational fluid dynamics code STAR-CCM+. Relevant boundary conditions between the domains were exchanged until acceptable convergence criteria had been achieved. The coupled codes were validated by simulating a transient experiment done in the TALL facility. During experiments, the mass flow rate was monitored. This mass flow rate was compared to that of the simulated mass flow rates. The mass flow rate obtained by the coupled codes correlated well with the experimentally measured mass flow rate and showed an improvement to the mass flow rate, calculated by the standalone RELAP simulation (Kööp, 2018). Several published 1D/3D co-simulation papers (Ampofo & Karayiannis, 2003; Kim, *et al*., 2014; Kööp, 2018; Lisowski, 2013) show a comparison with experimental setups, but few of them demonstrate how the co-simulation compares with 1D simulation on its own.

Du Toit, *et al*., (2014) and Rousseau, *et al*., (2015) considered an air-cooled RCCS and compared results obtained by the two different codes GAMMA+ and Flownex. Within the numerical simulations performed by Du Toit, *et al*., (2014) and Rousseau, *et al*., (2015) a temperature was specified as boundary conditions on the surface to represent the Reactor Pressure Vessel (RPV). A transient analysis was done using Flownex, in which the numerical model's sensitivity to flow reversals was tested. The analysis revealed that a reversal in flow direction was possible if the pressure increase on the outlet of the RCCS to atmosphere was high enough. Once flow reversal occurred within the system, the flow would not return to the original flow direction.

Flow reversal will have a detrimental effect on the reactor cavity structures, as a noticeable increase in temperatures was observed (Du Toit, *et al*., 2014). The authors concluded that this phenomenon needs to be considered when designing the system.

Within this paper, the behaviour of multiple 1D/3D co-simulation strategies are investigated by applying them to the radiative- and convective- heat transfer, and natural circulation phenomena occurring within a simplified water-cooled RCCS facility. Compared to flow systems where a fixed mass flow rate is prescribed, a natural circulating flow system can present additional stability challenges. The behaviour and validity of the coupled 1D/3D approaches are investigated by comparing them with a full 1D simulation of the simplified RCCS facility. The validity of the full 1D reference simulation is established by comparing the results predicted by the 1D simulation with the generalised correlation for steady-state turbulent flow in single-phase natural circulation loops (Vijayan et al., 2000).

2. 1D/3D Coupling Methodology

In the introduction, the need for developing a coupled methodology to perform a simulation combining a 1D systems code and a 3D CFD code was established. In this study, the thermal-hydraulic system's code Flownex (M-Tech Industrial, 2019b) is used as the 1D solver, while Ansys Fluent (Ansys, 2018) is used to calculate the 3D domain. Each code models a relevant part of the simplified RCCS facility. Typically, a 3D methodology was employed to model the radiation and convection heat transfer in the air-filled cavity between the heater wall and the outer wall of the riser. The 1D methodology was employed to model the remainder of the RCCS system which contained water as the coolant. The different models were coupled by explicitly exchanging boundary conditions or relevant data between the 1D and 3D regions.

2.1 One-dimensional simulation theory

Flownex, being a one-dimensional systems code and consisting of primarily dominant pipe flow during the co-simulation process, solves the one-dimensional conservations equations for mass, momentum, and energy. The general equation of mass conservation is written in a one-dimensional coordinate system in the following form

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho V) = 0 \tag{1}$$

In Eq. (1), V is the flow velocity in the x direction, i.e., along the length of the pipe element; ρ is the fluid density.

The momentum conservation equation for one-dimensional flow in a pipe can be written in the following form:

$$\frac{\partial(\rho V)}{\partial t} + \frac{\partial(\rho V^2)}{\partial x} = -\frac{\partial p}{\partial x} - \rho g \frac{\partial z}{\partial x} - \frac{f\rho|V|V}{2D} \tag{2}$$

The left-hand side of Eq. (2) contains the time derivative for transient flow and the convective term, while the right-hand side contains different forces acting on the control volume. The first term on the right-hand side is the pressure gradient source term and the negative sign indicates that the flow occurs from regions of high to low pressure. The second term is the body force due to gravity and the last term models the friction force due to shear stress. f is the friction factor calculated as a function of Reynolds Number for pipe flow and D is the diameter of the pipe.

Flownex SE employs the modified Colebrook-White correlation (Eq. 3) to determine the friction factor.

$$f = \frac{0.25}{\left[\log\left(\frac{\varepsilon}{3.7D} + \frac{5.74}{Re^{0.9}}\right)\right]^2} \tag{3}$$

The energy conservation for one-dimensional flow is expressed in terms of the specific stagnation enthalpy h_o as:

$$\frac{\partial(\rho(h_o+gz)-p)}{\partial t} + \frac{\partial(\rho V(h_o+gz))}{\partial x} = \dot{Q}_h - \dot{W} \tag{4}$$

The specific stagnation enthalpy is given by:

$$h_o = h + \frac{1}{2}V^2 \tag{5}$$

where the specific enthalpy h is given by:

$$h = u + pv \tag{6}$$

where v is the specific volume of the fluid. Du Toit (2021) demonstrated the ability of Flownex to accurately simulate steady-state behaviour of single-phase natural circulation loops with water as the coolant.

2.2 Three-dimensional simulation theory

Ansys Fluent makes use of the Finite Volume Method (FVM) to discretize the conservation equations for fluid flow (Ansys, 2017). This implies that the properties of mass, momentum, and energy are conserved locally over each Control Volume (CV). The Finite Volume Method (FVM) discretizes the flow domain into a finite number of non-overlapping Control Volumes (CV) with flat faces. The fundamental equations are then integrated over the control volumes to yield algebraic equations for the discretized variables such as temperature and velocity. A linearization of the algebraic equations is carried out to yield a matrix of linear equations of the discretized variables that are to be solved.

The 3D CFD governing equations (conservation equations for mass, momentum, and energy) are built into Ansys Fluent. The conservation of mass is given as follows (Ansys, 2017):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = S_m \tag{7}$$

The first term accounts for changes in mass due to transient effects, while the second term accounts for the movement of fluid over the control volume boundaries. The last term, S_m accounts for any additional mass sources added to the system.

The momentum conservation equation is given as (Ansys, 2017):

$$\frac{\partial}{\partial t}(\rho \vec{V}) + \nabla \cdot (\rho \vec{V}\vec{V}) = -\nabla p + \nabla \cdot (\bar{\bar{\tau}}) + \rho \vec{g} + \vec{F} \tag{8}$$

The first term accounts for momentum change during transients and the second term accounts for changes in momentum due to fluid moving over the boundary of the control volume. The third term accounts for the effect of a change in pressure on the momentum, the fourth accounts for the effect of the stress tensor, the effect of buoyancy and external forces are accounted for by the fifth and sixth terms respectively. ρ represents the density in [kg/m^3], $\vec{V}$ the velocity vector [m/s], p the pressure, g the gravitational acceleration [m/s^2] and $\vec{F}$ the external forces. ∇ is the operator for the partial derivative of the relevant quantity. The stress tensor, $\bar{\bar{\tau}}$ in Eq. (8) is given by

$$\bar{\bar{\tau}} = \mu\left[\left(\nabla\vec{V} + \nabla\vec{V}^{T}\right) - \frac{2}{3}\nabla\cdot\vec{V}I\right] \tag{9}$$

Where μ is the dynamic viscosity [kg/m-s] and I is the unit tensor.

The conservation of total energy, E is implemented in Ansys Fluent in the form (Ansys, 2017):

$$\frac{\partial}{\partial t}(\rho E) + \nabla\cdot\left(\vec{V}(\rho E + p)\right) = \nabla\cdot\left(k_{eff}\nabla T - \sum_j h_j\vec{J}_j + \left(\bar{\bar{\tau}}_{eff}\cdot\vec{V}\right)\right) + S_h \tag{10}$$

The first term accounts for energy changes due to transient effects, the second term for changes in energy due to fluid movement over control volume boundaries. The third term accounts for changes in energy due to conduction, diffusion, and viscous dissipation, respectively. S_h represents energy sources within a control volume. The effective conductivity, k_{eff} is a function of the thermal conductivity and the turbulent thermal conductivity [W/m-K]. T is the temperature measured in [K], h_j is the enthalpy, $\vec{J}_j$ is the flux at which a species j diffuses and $\bar{\bar{\tau}}_{eff}$ is the effective stress tensor.

To account for turbulent flow present within the coupled flow and heat transfer problem, a turbulence modelling scheme is used in conjunction with the conservation equations. Ji (2014) investigated the natural circulation in a square air cavity by comparing the results from different mesh sizes and turbulence models. The study included both 2D and 3D models with the k-ε, k-ω, RNG, and SST turbulence models. From the results gathered, the k- ω turbulence model performed the best overall in predicting the natural circulation phenomena. Therefore, the decision was made to implement the k- ω turbulence model within the 1D/3D co-simulations.

The k-ω SST model is formulated in Ansys Fluent as follows (Ansys, 2017a):

The equation for the kinetic energy, k:

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial X_i}(\rho k u_i) = \frac{\partial}{\partial X_j}\left(\Gamma_k \frac{\partial k}{\partial X_j}\right) + G_k - Y_k + S_k \tag{11}$$

The equation for the specific dissipation rate, ω:

$$\frac{\partial}{\partial t}(\rho\omega) + \frac{\partial}{\partial X_j}(\rho\omega u_j) = \frac{\partial}{\partial X_j}\left(\Gamma_\omega \frac{\partial\omega}{\partial X_j}\right) + G_\omega - Y_\omega + D_\omega + S_\omega \tag{12}$$

In Eq. (11) and Eq. (12), the first terms account for changes in the quantity due to transient effects, the second terms due to the transport of fluid over a given control volume. The third term accounts for the diffusion of the respective quantity, with G and Y representing generation and dissipation. S in the equations represent user-defined source terms where applicable. X_j represents the position within a reference frame. Γ is the effective diffusivity, while D_ω is the term accounting for cross-diffusion.

When modelling any CFD application, the appropriate use of wall functions is important. Wall functions reduce computational resources by approximating the velocities close to a wall, instead of directly modelling the velocity profile. y^+ is the non-dimensional distance from the wall to the first node in the mesh of the flow field next to the wall.

2.3 1D/3D coupling procedure and general coupling issues

As part of the Ansys Partner Ecosystem, Flownex has a built-in link to any Ansys fluid dynamics tool (Ansys, 2021). By modifying parameters and scheme variables within Fluent's User Defined Function (UDF) and Text User Interface (TUI), Flownex can be directly coupled with Ansys Fluent. This functionality allows users to solve 1D and 3D flows respectively by exchanging relevant data and information at the interface boundaries (Ansys, 2021; M-Tech Industrial, 2019a).

Successful co-simulation using Flownex and Ansys Fluent requires care in both coding and numerical modelling approaches. During the 1D/3D co-simulation solution process, principles of conservation need to be preserved at the interface between the 1D- and 3D- flow domains.

Explicit or semi-implicit coupling methodologies are available when coupling a thermal-hydraulic systems code and a 3D CFD code. The semi-implicit methodology requires that the data or relative information be transferred several times during each time-step until convergence of the coupled parameters is reached. The explicit methodology, as used within this study, requires that the data or relative information are exchanged between the different codes only once for each iteration.

Both node-averaged and boundary values can be explicitly transferred between Flownex and Ansys Fluent. The averaged values are calculated by using the appropriate volume, area, or density-weighted property depending on the mesh geometry or type of property.

Some generic issues to keep in mind when selecting the appropriate co-simulation methodology:

- Within the solution schemes, determine which phenomena will be calculated by which code.
- Different definitions of variables exist between Flownex and Ansys Fluent.
- The frequency in which data/information is transferred between the two codes.
- The method of time step control (in the case of transient simulations).

2.4 Solution Algorithm

M-Tech Industrial, (2019b) states that when using a coupled 1D/3D modelling process, transient simulations should be assumed to initiate from steady-state conditions. This will aid in reducing the time-consuming iterations between different codes until the 3D-domain solution converges.

Table 1 contains the solution strategies applied to the 3D Fluent domain. The SIMPLE (Semi-Implicit Method for Pressure Linked Equations) algorithm is used in all four 1D/3D co-simulation strategies. The algorithm is initialized by guessing an initial pressure field, which is then used to solve the discretized momentum equations. The solution to the momentum equations is then used to adapt the initial pressure. The corrected pressures are then used to re-calculate the velocity field. The other discretized transport equations are solved at this point where a convergence check can be done. The process is done iteratively until the required convergence criteria are met (Versteeg & Malalasekera, 2007).

Table 1: Solution strategies applied to the 3D (Fluent) domain

	Models/ Solution methodology applied
Turbulence model	k-ω SST model
Wall functions	Standard wall functions
Solution method	SIMPLE algorithm

The solution algorithm used for the four different 1D/3D co-simulation strategies is illustrated in Fig. 1. The solution algorithm starts by initializing both the Flownex- and Ansys Fluent- models and ensuring both cases/models can run separately in a stable manner through the use of fixed boundary conditions, i.e. uncoupled. Information transfer is initialized after steady-state solutions for the Flownex model are achieved. The communication link (Journal file/TUI) is established between the Flownex- and Ansys Fluent- model, whereby information or data transfer between the two codes can occur. An iterative procedure follows in which Flownex completes several iterations and transfers the necessary values to Ansys Fluent. Corresponding iterations are performed in Ansys Fluent after which the required parameters are sent back to Flownex. After this information transfer, the global iteration advances. This process is repeated until acceptable convergence criteria are reached within both Flownex and Ansys Fluent. The solution accuracy was deemed acceptable when the residuals and report definitions within Ansys Fluent were below $1e^{-05}$.

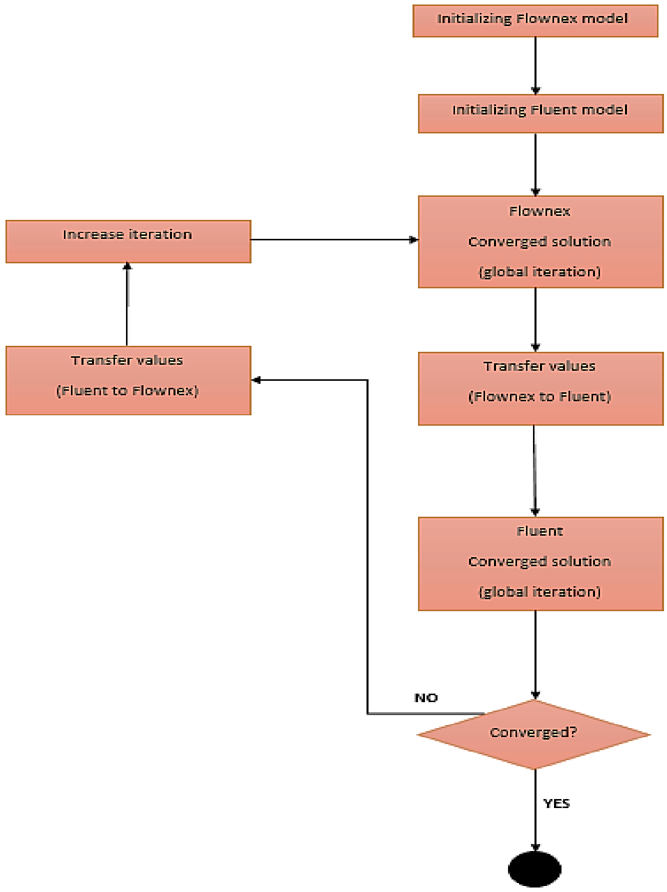

Figure 1: Solution algorithm for coupling Flownex and Ansys Fluent, Adapted from Source (Kruger & Du Toit, 2006).

3. Implementation of Coupling Methods

Four different 1D/3D co-simulation strategies exist when simulating an RCCS system which includes the Reactor Pressure Vessel (RPV) wall and cavity of the heater box; the risers; the inlet network and reservoir with associated heat removal system.

3.1 Model description

In the unlikely event of an accident scenario at a Nuclear Power Plant (NPP), Very High-Temperature gas-cooled Reactors (VHTRs) have several safety features. These safety features include safe fuel design (fuel contained within the TRISO-particles), low power density, negative temperature reactivity coefficients, and passive heat removal systems. The Reactor Cavity Cooling System (RCCS) is seen as an integral and crucial part of the passive safety concept associated with VHTR and Generation-IV reactors (Shin, *et al.*, 2017b). The system is intended to remove decay heat from the reactor cavity, passively without external inputs. According to IAEA (2000), the RCCS should be designed for efficient heat removal under accident conditions. However, during normal operation- and planned shutdown- conditions the system should not cause unnecessary heat dissipation. The accurate simulation of the radiative- and convective- heat transfer, as well as the natural circulation phenomena occurring within the RCCS facility, is therefore important to ensure reactor designs are passively safe (Shin, *et al*., 2017b).

The Reactor Cavity Cooling System consists of the following basic components, a cold down-comer, a hot riser, and a heat rejection zone. Coolant (typically water or air) is transported via downcomers to the hot risers, which are installed on the circumference of the reactor cavity. The number of risers installed varies, depending on reactor design. The thermal radiation- and convection- heat transfer from the Reactor Pressure Vessel (RPV) heats the coolant contained within the risers, resulting in a change in the coolant's density and therefore inducing the buoyancy forces that drive the system. As the heated coolant moves upward and out of the risers, heat rejection occurs either through a heat exchanger or to the atmosphere.

A conceptual illustration by Shin *et al*. (2017a) of an air-cooled RCCS is shown in Fig. 2. The figure illustrates the heat transfer from the Reactor Pressure Vessel (RPV), which leads to the development of the natural circulation phenomena occurring within the ducts of the RCCS.

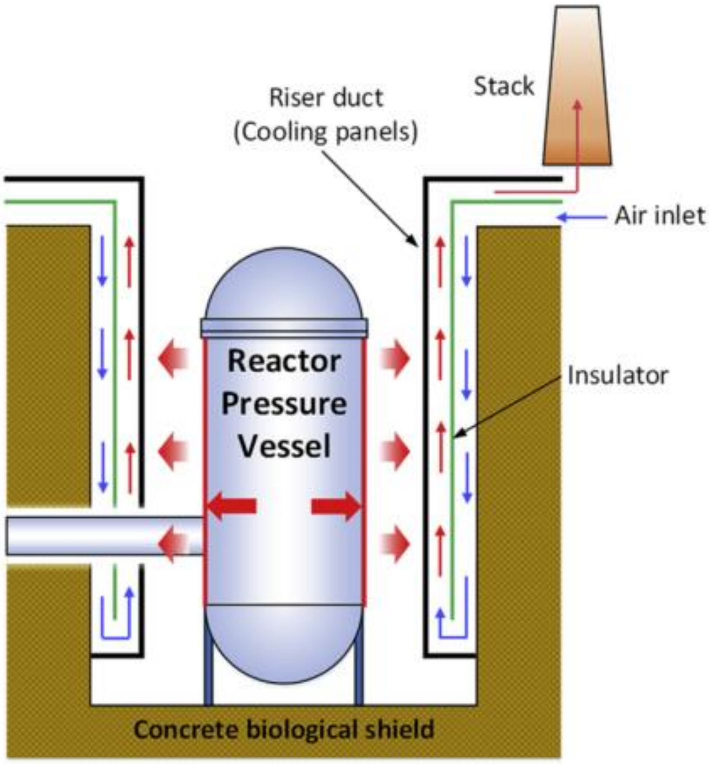

Figure 2: Conceptual depiction of the RCCS (Shin, *et al.*, 2017a)**.**

Fig. 3 illustrates a schematic representation of the simplified water-cooled Reactor Cavity Cooling System (RCCS) facility being simulated. The RCCS model consists of a reservoir (water tank), downcomer, lower pipe network, heater box (Fig. 3), and chimney. The reservoir is divided into three sections, i.e., an upper reservoir from the inlet of the chimney to the water level, a middle reservoir with length 0.3 [m], and a lower reservoir from the bottom of the middle reservoir to the outlet at the bottom of the tank. Within the 1D/3D co-simulation, the middle reservoir is used to fix the cold flow temperature in the absence of the air-cooled heat exchanger loop. The datum level of the geometry is taken to be the centreline of the lower network (i.e., a lower inlet in Fig. 3).

The upper node of the upper reservoir (Point 1) represents the water level in the reservoir and a total pressure of 100 [kPa] is specified at this point. Due to the layout (and the incompressible nature of water), the mass flow rate within the upper reservoir will be zero.

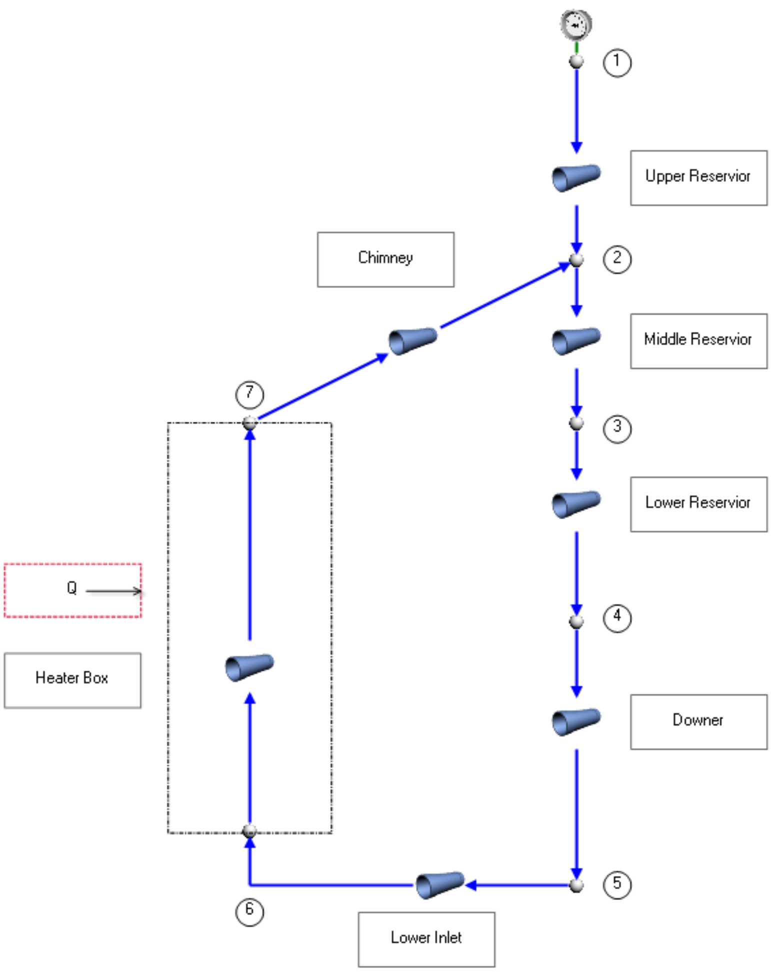

Figure 3: Schematic representations of the simplified water-cooled RCCS system.

In terms of the description given by Vijayan *et al*. (2000) the layout shown in Fig. 3 is considered to be a vertical heater vertical cooler (VHVC) configuration.

The heater box (Fig. 4) consists of the heater wall, air cavity, and riser pipes/tubes. Top and bottom end caps of thickness 0.005 [m] were added to the heater box cavity. Table 2 contains the geometrical properties associated with the integrated RCCS components. The roughness of all the components was taken to be 15 [μm].

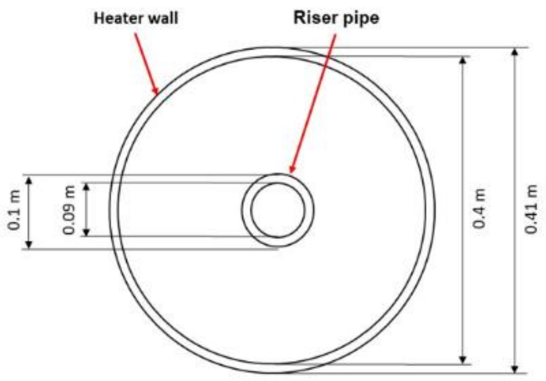

Figure 4: Heater Box.

Table 2: Geometrical properties.

Location	Description	Length	Diameter	Elevation
Point [1]	Upper Reservoir	0.7 [m]	0.91 [m]	6.8 [m]
Point [2]	Middle Reservoir	0.3 [m]	0.91 [m]	6.1 [m]
Point [3]	Lower Reservoir	0.5 [m]	0.91 [m]	5.8 [m]
Point [4]	Downer	5.3 [m]	0.10 [m]	5.3 [m]
Point [5]	Lower Inlet	2.0 [m]	0.10 [m]	0.0 [m]
Point [6]	Heater Box	5.0 [m]	0.09 [m]	0.3 [m]
Point [7]	Chimney	2.0 [m]	0.10 [m]	5.3 [m]

Lisowski (2013) performed both single-phase and two-phase tests using the experimental UW-RCCS facility. The relevant data of the selected single-phase steady-state test are given in Table 3 and serve as input specifications used within this study.

Table 3: Data of single-phase steady-state test (Lisowski, 2013)**.**

	Run007
Riser power [kW]	3.778
Inlet Temperature [C]	30.00
Outlet Temperature [C]	32.67
Mass flow rate [kg/s]	0.37

A full 1D simulation (Fig. 5) was created in Flownex to simulate the radiative- and convective- heat transfer, and natural circulation phenomena occurring within the simplified RCCS facility. The conduction heat transfer through the heater- and riser walls was modelled using two conduction components (HW and RW) respectively. Radiation was assumed to be the dominant heat transfer mechanism in the cavity and convection heat transfer in the cavity was therefore not included in the model. A surface-to-surface radiation component (CA) was used to model the radiative heat transfer between the heater- and riser wall. A convection component (CO) was used to model the convection heat transfer between the riser wall and the water flowing within the riser. The convective heat transport and flow in the riser were modelled using a pipe component.

The local loss coefficients associated with the lower inlet (LI), heater box (HB) and chimney (CH) were assumed to be 2.0, 6.6 and 1.2 respectively and were chosen to ensure the required steady-state mass flow rate. The local loss coefficients associated with the other components were assumed to be zero.

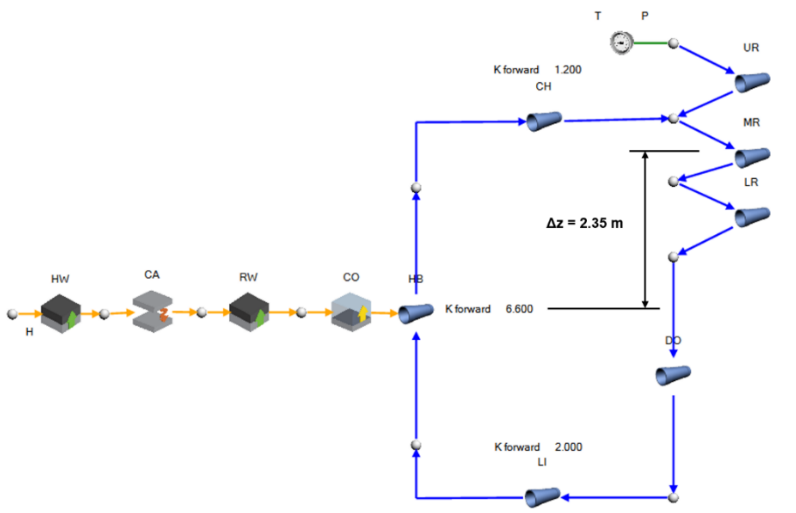

Figure 5: Flownex network of the full 1D RCCS simulation

3.2 Case descriptions:

[1] The first approach can be described as a **directly coupled inline** (domain decomposition) model. The entire test section (heater box) is modelled in 3D, whilst the remainder of the system is modelled in 1D. At the outlet of the lower manifold (lower inlet in Fig. 3) the 1D code provides the 3D code with the mass flow rate and the temperature of the water, whilst at the outlet of the heater box in Fig. 3, the 1D code provides the 3D code with the pressure. The 3D code in turn provides the 1D code with the pressure at the outlet of the lower inlet and the water temperature at the outlet of the Heater box.

[2] The second approach can be described as a **directly coupled parallel** model. The outside wall of the heater box, air-cavity/cavities in the heater box, and the wall of the riser tubes in the heater box are modelled in 3D. The fluid flow in the pipe network, risers and the remainder of the system is modelled in 1D. The 3D code provides the 1D code with the heat flux/heat transfer rate at the inside surfaces of the riser tubes, whilst the 1D code provides the 3D code with the temperatures of the inside surfaces of the riser tubes.

[3] The third approach can be described as an **indirectly coupled parallel** (domain overlapping) model. As in the first approach the entire test section is modelled in 3D. As in the second approach, the fluid flow in the pipe network, risers and the remainder of the system is modelled in 1D. The 1D code provides the 3D code with the mass flow rate and the temperature of the water at the inlet of the lower inlet, as well as the pressure at the outlet of the Heater box. The 3D code only provides the temperature of the water at the outlet of the Heater box to the 1D code.

[4] The fourth approach can be described as an **indirectly coupled parallel** (flow resistive component) model. Again, the entire test section is modelled in 3D. The remainder of the system is modelled in the 1D model as in the other models, whilst the flow in the risers is modelled using a flow resistance component which uses a representative resistance to determine the pressure drop over the test section. At the inlet of the lower inlet, the 1D code provides the 3D code with a mass flow rate and temperature of the water, whilst at the outlet of the heater box the 1D code provides the 3D code with the pressure. The 3D code in turn provides the 1D code with the pressure at the inlet of the lower inlet and the water temperature at the outlet of the heater box. The outlet pressure provided by the 1D code and inlet pressure obtained by the 3D code is then used to recalibrate the resistance of the flow resistance component before proceeding with the next global iteration.

The pressure drop over the flow resistance component is given by:

$$\Delta p_0 = \frac{\dot{m}\,|\dot{m}|}{A_i A_o} + \rho g \Delta z \tag{13}$$

with A_o the flow-area and A_i the admittance, to be calculated, in order to give the pressure drop as calculated by the 3D model.

Approaches 1, 3 and 4 also require the 3D discretization of the flow in the risers accounting for the large difference between the number of cells required in approaches 1, 3, and 4 compared to the number of cells required in approach 2 as can be seen in Table 5.

The purpose of the study is to evaluate the performance of the coupled 1D/3D approaches based on the steady-state natural circulating flow in the selected simplified RCCS facility to determine the most promising 1D/3D coupling approach to simulate natural circulating flows. The validity of the results predicted by 1D/3D approaches is determined by comparing them with the corresponding results of the full 1D simulation of the simplified RCCS facility. The intention is to evaluate the characteristics of the most promising 1D/3D coupling approach to simulate natural circulating flows in greater depth by applying it to more complex RCCS configurations and fully transient situations in future studies.

A summary of the transmitted data between Flownex and Ansys Fluent and vice versa is given in Table 4:

Table 4: List of transmitted data.

	Flownex → Ansys Fluent	**Ansys Fluent → Flownex**
Approach [1]	$\dot{m}$; T_{in} ; P_{out}	P_{in} ; T_{out}
Approach [2]	$T_{surface}$	$\dot{Q}$
Approach [3]	$\dot{m}$; T_{in} ; P_{out}	T_{out}
Approach [4]	$\dot{m}$; T_{in} ; P_{out}	P_{in} ; T_{out}

The 3D geometry of the heater box (Fig. 4) was assembled in Solidworks (Dassault Systems, 2017) and imported into Ansys Fluent. A tetrahedral sweep- and assembly- meshing scheme was used to ensure that the cell faces on the interfaces between adjacent parts and assemblies matched to form a conformal mesh throughout the entire model. In Ansys Mesher, inflation regions were created on the heater- and riser-wall(s) (inner and outer walls) depending on the 1D/3D co-simulation approach being investigated. The inflation regions were created on the wall faces to propagate the prism layers from. Five prism layers were specified and the layer thickness of all the layers was chosen such that each layer stretched by a factor of 1 and the total thickness of the combined five layers was 0.4 [mm].

All the calculations were performed on a workstation computer with the following hardware specifications. Intel ® Xeon ® Gold 6140 CPU rated @ 2.30 GHz, 128 GB 2666 MHz RAM, and NVIDIA Quadro P400 GPU. This computer was sufficiently powerful to run all simulations, in particular the 3D iterations, in a reasonable amount of time.

3.3 Validation of Flownex simulation

To establish the validity of the result of the Flownex reference simulation, the results of a set of selected simulations will be compared with generalized correlation by Vijayan *et al.* (2000) for the steady-state Reynolds number Re_{ss} for natural circulating turbulent flow:

$$Re_{ss} = 1.96\left[\frac{Gr_m}{N_G}\right]^{0.364} \quad (14)$$

In the current study, the value of Re_{ss} is taken as $Re_{ss} = Re_{HB}$, e.g., the value of the Reynolds number in the riser pipe in the heater box. The value of the modified Grashof number Gr_m is obtained from (Vijayan *et al.*, 2000):

$$Gr_m = \frac{D^3\rho^2\beta g\dot{Q}\Delta z}{\mu c_p A} \quad (15)$$

Where β is the volumetric expansion coefficient of the water, Δz the vertical distance between the middle of the riser pipe in the heater box and the middle reservoir that serves as the heat exchanger as indicated in Fig. 5 (Vijayan et al., 2000), and c_p is the specific heat capacity of the water. The values of the water properties are taken at the average water temperature in HB, which is representative of the average water temperature in the loop. The value of the geometric parameter N_G is calculated as (Vijayan *et al.*, 2000):

$$N_G = \sum_{i=1}^{n}\left[\frac{L_i}{D_i} + \frac{K_i}{f_i}\right] \quad (16)$$

Where $n = 6$ are the number of active pipe components in the loop, L_i the length of pipe i component and K_i the local loss coefficient associated with pipe i.

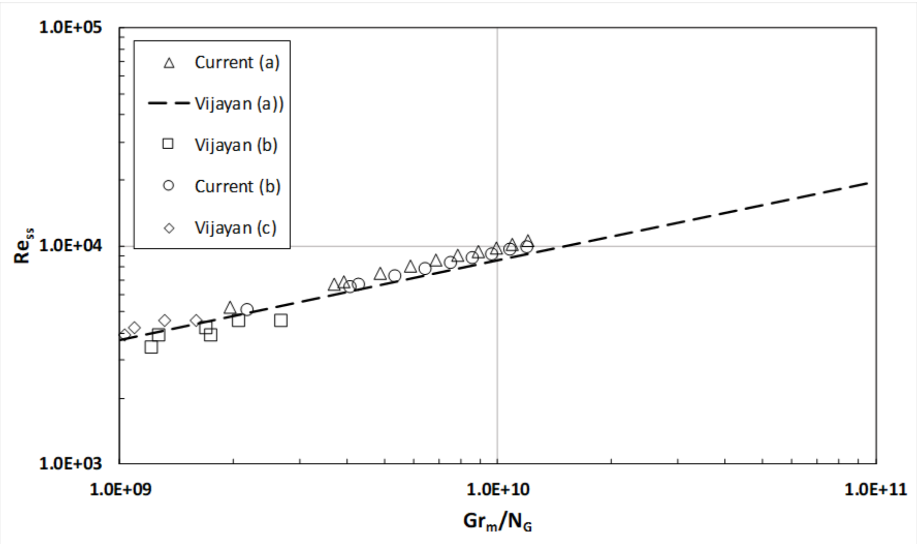

Figure 6: Comparison of the 1D Flownex simulation data with the correlation and experimental results of Vijayan *et al*. (2000)

In Fig.6 results obtained from the 1D Flownex model are compared with the generalised correlation for turbulent flow of Vijayan *et al*. (2000), Eq. (14), depicted as Vijayan (a) in Fig. 6. Two sets of results obtained by the Flownex model are shown in Fig. 6, i.e., Current (a) and Current (b). Current (a) are the results for the configuration, Fig. 5, as discussed in section 3.1. Note that all the loop pipe components do not have the same diameter. Current (b) are the results that are obtained when all the loop pipe components have the same diameter, namely 0.1 m. Vijayan (b) are the experimental results for an VHVC configuration obtained by Vijayan et al. (2000) when local losses are not accounted for, whilst Vijayan (c) are the corresponding results when local losses are accounted for. The experimental loop had an inner pipe diameter of $D = 0.0269\ m$ and a total length of $L_t = 7.18\ m$. It can be observed in Fig. 6 that the agreement between the current results, the generalised correlation of Vijayan *et al.* (2000) and the experimental results of Vijayan *et al.* (2000) is good. The good agreement can be considered as a validation of the 1D Flownex model and that the results obtained by the model can, therefore, be used as a reference solution.

4. Results and discussions

The four different 1D/3D co-simulation strategies were implemented to simulate the radiative- and convective- heat transfer as well as the natural circulation phenomena occurring in the simplified RCCS facility **(**Fig. 3**)**. The validity of the different 1D/3D co-simulation approaches is investigated by comparing their results with the results obtained by the full 1D simulation of similar specifications and setup. These strategies were evaluated based on simulation- stability, -time, and results.

Table 5 illustrates a side-by-side comparison of the relevant results for both the full 1D analysis and the 1D/3D co-simulation approaches. The following remarks can be made for the four different 1D/3D co-simulation strategies investigated:

(i) *directly coupled – inline/series*: Within this strategy, the 1D solver models the entire system, except for the area of the simulation that would greatly benefit from the increased detail of 3D CFD (e.g., the heater box). The systems code is directly connected to the inlet and outlet of the 3D CFD model.

The disadvantage of using this coupling method would be instability caused, by the direct series coupling, as evident from the diverging nature of the solution results as once flow reversal occurred within the system, the flow would not return to the original flow direction. The initial boundary values as input conditions in both Flownex and Ansys Fluent networks should have similar values to ensure any numerical discrepancy between the Flownex and Ansys Fluent networks is minimized. This method is the most explicit and will result in a long solution time, as the 1D/3D co-simulation approach is based on a systems-level only. For the RCCS setup considered this approach required the largest number of iterations to obtain convergence. However, the solution time is the second largest.

(ii) *directly coupled – parallel*: Similar to the directly coupled – inline/series strategy, the entire system is modelled using the 1D systems code, Flownex. However, the area of the simulation that would greatly benefit from the increased detail of 3D CFD, is modelled using both Ansys Fluent and Flownex. This method allows for part of the 3D domain to be solved using the 1D systems code.

The flow within the riser was simulated in Flownex. This required that both the Flownex and 3D Ansys Fluent model be divided into axial increments. This allowed for better heat input distribution per increment, to allow for more detailed 3D results to be obtained from the coupled 1D/3D simulation. This model uses only the convection and pipe elements and their corresponding nodal elements to represent the flow and convection heat transfer in the riser. The boundary conditions at the inlet and outlet of the heater box were the same as the corresponding boundary conditions used within the full 1D simulation. Even though this method may be time-consuming to set up, a noticeable reduction in computational resources can be observed. This method is robust and solves relatively quickly when compared to the other 1D/3D co-simulation strategies. For the RCCS setup considered this approach required the least number of iterations to obtain convergence and also had the shortest solution time.
The difference in the outlet temperature needs to be investigated further. It may be attributed to the fact that in 1D simulation the riser is discretized much finer, resulting in a more detailed distributed application of the heat flux and the calculation of water properties. In the full 1D simulation and approaches 3 and 4, only one increment is used in the 1D simulation to model the riser. In approach 1 the riser is not modelled in the 1D model.

(iii) *indirectly coupled – parallel (domain overlapping):* Unlike the directly coupled-parallel strategy, the heat transfer mechanism and fluid flow present within the risers are solved by both codes simultaneously. Ansys Fluid transfers an outlet temperature to Flownex. Data transferred to Ansys Fluent from Flownex, will then be an inlet mass flow rate, inlet temperature, and outlet pressure. Within this method, the interchange of information leads to the calibration of the buoyancy force to obtain the mass flow rate for which the system is in thermal equilibrium. This method may be favoured as setting up the simulation would be less time-consuming than that of the directly coupled -parallel strategy. Also, the discrepancies that hinder the directly coupled – inline/series strategies are easier to detect as both Flownex and Ansys Fluent generate boundary conditions on a feedback loop. This method is, however, not without major drawbacks, as significant computational resources are required. The analysis also revealed that a reversal in flow direction was possible if the pressure increase on the outlet of the RCCS to atmosphere was high enough. Once flow reversal occurred within the system, the flow would not return to the original flow direction. Special attention in the solving strategy is therefore needed to reach a converged solution.

(iv) *indirectly coupled – parallel (flow resistive component):* This configuration is similar to the indirectly coupled -parallel strategy, with the exception that the fluid flow within the risers in the 1D simulation is modelled using Flownex's flow resistance component. The flow resistance component calculates the flow resistance (admittance) of the 3D model based on the in- and outlet pressures,

gravitational force, and mass flow rate. In the simulations the values of the flow area (A_o) and admittance scaling factor (A_i) opening are assumed to be unity.

This strategy works well when representing a complex geometric component that would otherwise be difficult to represent in a 1D system code. However, this co-simulation has limitations in its ability to solve complex heat transfer problems. This strategy is prone to diverge due to flow reversal, as seen by the large solution time. To help alleviate the divergence experienced, a time-consuming iterative boundary conditions update methodology needs to be adopted.

Table 5: Results comparison

	1D Simulation	1D/3D Co-simulation approach			
	Full 1D	Approach [1]	Approach [2]	Approach [3]	Approach [4]
Riser Power [kW]	3.778	3.778	3.778	3.778	3.468
Inlet Temperature [C]	30.25	30.25	30.25	30.25	30.25
Outlet Temperature [C]	32.67	32.497	31.87	32.245	32.04
Mass flow rate [kg/s]	0.37	0.37	0.3702	0.37	0.3
Number of cells [-]	-	8 387 548	4 842 632	8 687 608	8 687 608
Number of iterations [-]	102	5 400	980	5 200	4400
Solution time [s]	0.19	20 860	2643	19 380	34 580

5. Conclusions

Four different co-simulation approaches were explored to investigate the radiative- and convective- heat transfer, and natural circulation phenomena occurring in a simplified water-cooled RCCS facility. The impact on simulation- stability, -time, and results are investigated to help serve as a basis for future 1D/3D co-simulation implementations. Flownex and Ansys Fluent each modelled a relevant part of the RCCS facility, and the models were explicitly coupled by exchanging boundary conditions between the models/codes. The 1D/3D co-simulation methodologies were compared to a full 1D model consisting of the same specifications and setup. It was found that the related temperatures, mass flow rates, and riser power for all four co-simulation strategies were in good agreement with the results obtained from the full 1D simulation.

The directly coupled–parallel strategy is the preferred method of choice due to the fact that it requires less computational resources and reaches a converged solution in the least number of iterations and amount of solution time. This despite the fact that it could be time-consuming to set up a model.

The directly coupled -inline strategy would be the second method of choice, as some areas of a system/component cannot always be characterized in a representative 1D manner that requires less detail than that of a full 3D simulation. This method will yield a converged solution in a reasonable amount of time.

CRediT authorship contribution statement

O.C. Koekemoer: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Writing – Original Draft, Project administration.

Prof. C.G. du Toit: Conceptualization, Supervision, Software, Writing – review and editing. Project administration.

P.F. Niemand: Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Nomenclature
Abbreviations

1D	One –dimensional
3D	Three -dimensional
CFD	Computational Fluid Dynamics
CV	Control Volume
FVM	Finite Volume Method
NPP	Nuclear Power Plant
PRHRS	Passive Residual Heat Removal System
RCCS	Reactor Cavity Cooling System
RNG	Re-Normalization Group
RPV	Reactor Pressure Vessel
SIMPLE	Semi-Implicit Method for Pressure Linked Equations
SST	Shear Stress Transport
TRISO	Tri-structural-isotropic
TUI	Text user interface
UDF	User defined function
UW	University of Wisconsin
VHVC	Vertical Heater Vertical Cooler
VHTR	Very High Temperature gas-cooled Reactor

List of Symbols

∇	Gradient
A_o	Flow area
A_i	Admittance
β	Volumetric expansion coefficient
Cp	Specific heat
D	Diameter
E	Energy
f	Friction factor
F	External force

G	Generation
Gr	Grashof Number
g	Gravitational acceleration
h	Enthalpy,
I	Unit tensor
J	Flux
k	Conductivity
K	Kelvin, Local heat loss coefficient
L	Length
ṁ	Mass flow rate
N	Geometric parameter
Nu	Nusselt Number
μ	Dynamic viscosity
ω	Omega, specific dissipation rate
P	Pressure
Q	Heat transfer rate
ρ	Density
Pr	Prandtl Number
Q	Heat transfer rate
Γ	effective diffusivity
Re	Reynolds Number
S	Source term
τ	Shear stress
T	Temperature
t	Time
v	Specific volume
V	Mean velocity
u	Velocity, internal energy
x	Direction
Y	Dissipation
z	Elevation, direction

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4. ARTICLE 3: SIMULATING HEAT TRANSFER IN A PRISMATIC BLOCK VHTR USING A 1D/3D CO-SIMULATION METHODOLOGY

Abstract:

The VHTR's inherent safety, high thermal efficiency, and high reactor outlet temperature of as high as 1000 °C has led to the development and implementation of VHTRs in process heat, hydrogen production, and power generating applications. These reactors require effective and demonstrable computational tools and methodologies for the design-, operation-, and safety analyses. However, simulating the thermal-hydraulic behaviour in prismatic block reactor units poses several challenges and typically requires significant computational resources and computational times. The numerical models of prismatic block reactors must amongst others account for the thermal-fluid phenomena in the fuel compacts, graphite, coolant channels in the fuel blocks, bypass and cross gaps between fuel blocks and the mixing in the upper and lower plenums. Due to the limitations on available computing power, this amount of detail cannot be accounted for in a single explicit three-dimensional numerical model. This paper describes the development of a methodology that couples a one-dimensional (1D) systems code and a three-dimensional (3D) Computational Fluid Dynamic (CFD) code. By combining the desired features of a one-dimensional systems code and a three-dimensional CFD code, the required resources are optimized whilst still retaining an acceptable level of accuracy. The 1D/3D co-simulation methodology is demonstrated by simulating the heat transfer and fluid flow within a single-channel fuel module of a prismatic block VHTR. In the coupled 1D/3D model, the one-dimensional (1D) elements represent the tube flow within the coolant channels while the spatial elements represent the fuel-compact and graphite moderator associated with a single-channel fuel module. The coupled 1D/3D methodology was validated against corresponding values obtained from published work as well as full CFD. The coupled 1D/3D models indicate errors between the calculated fuel- and coolant temperatures for both a (i) uniform, and (ii) cosine power profile of less than 1.5%, when compared to a full CFD analysis of the same system. By explicitly coupling the 1D and 3D solvers the computational expense is greatly reduced when compared to full CFD. Therefore, the coupled 1D/3D methodology can form the basis of an integrated model for the entire prismatic core.

Keywords:

One-dimensional (1D), three-dimensional (3D), coupled 1D/3D modelling, Computational Fluid Dynamics (CFD), Very High Temperature Reactor (VHTR), heat transfer.

1. Introduction

The Very High Temperature gas-cooled Reactor (VHTR) is one of six nuclear reactor systems currently being investigated and implemented within the nuclear industry (GIF, 2014; Shin, *et al*., 2017). These six reactors with improved safety concepts form part of the so-called Generation IV technologies. The VHTR is a graphite-moderated helium-cooled reactor with a thermal neutron spectrum and a core design consisting either of a packed pebble bed or prismatic blocks. According to Hicks (2011), a prismatic core consists of an inner reflector region surrounded by an annulus of fuel blocks which in turn is surrounded by an annulus of outer reflector elements. The fuel blocks consist of hexagonal columns of graphite with circular holes that run the full length of the column. Fuel compacts consisting of TRISO (Tristructural-isotropic) particles are contained within the fuelled holes, while the coolant holes align axially to form coolant channels. In a pebble bed core, the TRISO particles are surrounded by an 'overcoat' of a carbonaceous material pressed together to form fuel pebbles which are stacked within a graphite reflector structure (Tak, *et al*., 2008).

During the normal operation of the VHTR, heat is generated by the fission reactions in the reactor core and is removed by the forced circulation of helium as it flows within the core. A portion of this heat is not removed and penetrates the structures within the reactor building. The reactor building is surrounded by a wall of concrete which is reported to become brittle at temperatures exceeding 65°C (Dilling, *et al*., 1982). Therefore, it becomes imperative to remove this heat to protect the concrete biological shield from overheating. In both prismatic block and pebble bed configurations, helium is collected within the upper plenum and flows downward into the core. In a prismatic core, the helium-coolant follows a well-defined path through the coolant channels. In the prismatic design, there is an undefined quantity of bypass flow as the flow moves between fuel blocks. However, in a pebble bed, helium coolant follows a multi-dimensional path defined by the voids between the pebbles (Hicks, 2011).

One of the challenging design issues in the development of the VHTR is an undesirably high nuclear fuel temperature within the prismatic core. This high temperature affects the integrity of the TRISO particles as well as the fission products released (Tak, *et al*., 2008). The higher-than-normal fuel temperature is furthermore directly related to the increased core outlet temperature of the VHTR. To adhere to the widely accepted design limit (~1250 °C) for TRISO particles, the maximum temperature difference between the coolant and the nuclear fuel should be less than ~ 250 °C (Collins, 2009; IAEA, 1990).

Considering the non-uniform power distribution in the reactor core as well as the low heat transfer characteristics of the helium-coolant, the fuel temperature limit is a crucial design criterion/issue for VHTRs. Understanding the thermal behaviour and predicting accurate coolant- and fuel temperatures is thus of considerable importance in the design of VHTRs.

Several phenomena exist that either directly or indirectly impact the thermal-hydraulic analysis of both the pebble bed and prismatic block VHTR systems. However, within this study, the focus will be on prismatic block VHTRs and the thermal-hydraulic analysis thereof.

The high heat capacity associated with the core structures of gas-cooled reactors play an important role in the transient response of the system. High leakage flow rates of the helium-coolant can occur as it is impossible to perfectly seal the gaps in between the graphite fuel and reflector blocks. The presence of cross- and bypass gaps poses several challenges as an intricate network of parallel and series flow paths through the reactor core structures develop. The presence of these gaps should be accounted for in the analysis of pressure drop and heat transfer characteristics. Helium is also prone to thermal stratification and therefore special attention is required to ensure sufficient mixing in plenums within the reactor occurs.

Modelling prismatic block high-temperature gas-cooled reactors units in full detail, therefore, poses tremendous challenges and typically require significant computation times and computational resources. This is largely due to the complexity of prismatic block reactor models as these models must amongst others account for the thermal-fluid phenomena in the fuel-compacts, graphite, and coolant channels in fuel blocks, cross- and bypass gaps between blocks and the mixing in the upper and lower plenums. According to Zhen (2008), the thermal-hydraulic behaviour of a VHTR can be analysed by either using a systems code, or any Computational Fluid Dynamics (CFD) code capable of modelling normal operation- and/or severe accident scenarios. Nuclear systems codes such as CATHARE (IRSN, 2006), Flownex SE (M-Tech Industrial, 2019b), and RELAP5 (INL, 2018) are widely used to investigate the thermal-hydraulic characteristics of nuclear power plants (NPPs) either under normal steady-state conditions or during various accident scenarios. Computational fluid dynamics codes such as Ansys CFX (Ansys, 2017), Ansys Fluent (Ansys, 2017), and STAR-CCM+ (CD-adapco, 2015) are also widely employed in nuclear reactor safety and design to analyse important 3D effects where greater detail about thermal interactions are required.

Three-dimensional (3D) CFD has advantages in that these codes can model the presence of localized hot spots and areas where greater detail about thermal interactions is required. The downside is the computational expense required in relation to the size and complexity of the problem under investigation. A one-dimensional (1D) systems code can also be used to analyse the fluid flow present but lacks detailed flow field predictions when compared to that of a 3D CFD analysis. Several contributions and models used to address the challenges encountered in the analysis of gas-cooled HTR systems can be found in the open literature. These vary in level of detail from systems models capable of simulating the full reactor unit using a 1D implicit approach, to explicit 3D models used to simulate a selected component or section of the reactor unit.

Johnson *et al*., (2012) and Tak *et al*., (2008) modelled the fuel compacts, graphite, coolant channels and bypass gaps of 1/12th of a fuel assembly in explicit detail. Both Johnson *et al*., (2012) and Tak *et al*., (2008) applied specified prescribed power profiles and investigated the effect of bypass gap size on the thermal-flow behaviour of fuel assemblies. Johnson *et al*., (2012) used the CFD code Ansys Fluent to model 1/12th of a GT-MHR fuel assembly, whilst Tak, *et al*., (2008) modelled 1/12th of a PMR600 fuel assembly using the CFD code CFX. Tung *et al*, (2013, 2016) also modelled 1/12th of a fuel assembly in STAR-CCM+ and studied the natural circulation that occurs after a loss of flow accident.

Lee *et al*., (2016) and Yoon *et al*., (2012) used explicit 3D detail to simulate the flow in the coolant channels, bypass gaps and cross gaps of an iso-thermal fuel block assembly. Lee, *et al*., (2016) characterized the pressure over a cross gap to obtain a correlation that can be implemented within a 1D systems/network code, whilst Yoon, *et al*., (2012) investigated the effect of variable bypass gap sizes. Both Lee, *et al*., (2016) and Yoon, *et al*., (2012) compared measured experimental results to those obtained from their respective CFX simulations.

Travis & El-Genk (2013a) investigated the thermal flow in a single fuel- and single control block. The authors used explicit 3D detail to simulate the flow paths and solid conduction elements, considering both bypass- and no bypass-flow. The calculated results were compared to simulations in which the flow paths were calculated using a 1D approach and the solid conduction was modelled in 3D detail. The results were found to be in good agreement. Subsequently, Travis & El-Genk (2013a) modelled 1/6th of a core using 3D detail for the solid conduction and the 1D approach for the coolant channel and bypass gaps and control rod flow. However, no description of the methodology as to how the convection heat transfer coupling between the 1D fluid flow and the 3D heat transfer was implemented was given.

Tak, *et al.*. (2012) and Tak, *et al.*, (2014) described the development of the CORONA code for the analysis of the heat transfer and fluid flow in prismatic block VHTR cores. The code uses an implicit 1D formulation to model the flow in the coolant channels, bypass gaps, and cross gaps whilst an explicit 3D formulation is used to model the heat transfer in the solid fuel-compact and graphite moderator. The results obtained were found to be in good agreement with results obtained from 3D explicit detailed simulations using the CFD code CFX. Tak, *et al.* also used this 3D/1D approach employed within CORONA to model the thermal flow in a 1/6th sector of a core which included the inner and outer reflector blocks and the riser holes. Lee *et al*., (2014) used CORONA software to investigate the effect of coolant channel blockages in 1/12th of a fuel assembly and compared the 3D/1D results with those obtained from a 3D explicit CFD simulation. The authors reported that the 3D/1D results were in good agreement. This led to the authors using CORONA to study the effect of heat transfer and flow in 1/6th of a core for single and multiple coolant channel blockages.

Cioni, *et al*., (2006) used the CFD code Trio_U to simulate the effect of selected coolant channel blockages on the temperature distribution in a prismatic fuel block of a VHTR. The flow in the coolant channels, as well as the bypass gaps, were modelled using a 1D approach, whilst the heat transfer phenomena within the fuel compact and graphite moderator were modelled using an explicit 3D approach.

Kim and Lim (2011) studied the effect of various bypass gap and cross gap sizes on the thermal flow in $1/6^{th}$ of a core using the 1D/2D/3D systems code GAMMA+. The fluid flow and heat transfer in the fuel blocks were modelled implicitly and a 1D approach was used to simulate the flow in the cross- and bypass-gaps.

Maruyama *et al*. (1993) and Maruyama *et al*. (1994) described the thermal-flow behaviour of the High-Temperature Test Reactor (HTTR) using a combination of a systems code and a 2D axisymmetric network code. The flow in the coolant channels, bypass gaps and cross gaps were modelled using the systems code FLOWNET. The 2D axisymmetrical network code TEMDIM was employed to calculate the heat transfer in the graphite and fuel compacts. Rousseau and Greyvenstein (2002) used the systems code Flownex, and also employed a 2D axisymmetrical network model to simulate the thermal-hydraulic behaviour of the HTTR. Rousseau and Greyvenstein (2002) however, only considered the flow in the coolant channels and the heat transfer through the fuel and reflector blocks.

When coupling an explicit 3D model and 1D model to simulate the heat transfer in the solids (fuel compact and graphite moderator) and the fluid flow in the coolant channels respectively, the use of an appropriate convection heat transfer correlation is required. Travis & El-Genk (2013b) used the CFD code STAR-CCM+ to perform a 3D explicit detailed simulation of a single-channel fuel module (SCFM) to evaluate various heat transfer correlations. The authors then proposed and implemented an improved convection heat transfer correlation into a coupled 3D/1Dsimulation of the SCFM. The 3D heat transfer was modelled using STAR-CCM+. However, no information regarding the 1D formulation used was given.
The contributions reviewed, show the limitation of the explicit 3D approach to model an entire reactor core unit. In none of the coupled 3D/1D simulations reported in the literature, any description is given in the way in which the convection heat transfer coupling between the 3D heat transfer and 1D fluid flow was implemented.

Recognizing the limitations on available computing power, this paper is aimed at combining the desired features of a one-dimensional systems code and a three-dimensional CFD code to simulate the heat transfer and fluid flow within a single-channel fuel module of a prismatic block VHTR. The one-dimensional (1D) systems code, Flownex, and the three-dimensional (3D) CFD code Ansys Fluent was used to perform the coupled 1D/3D simulations.

Within the coupled 1D/3D models, the 1D elements represent the flow within the coolant channels while the spatial elements represent the fuel-compact and graphite moderator associated with the single-channel fuel module. Koekemoer *et al* (2019) first constructed a coupled 3D and 1D model to simulate the heat transfer in a single-channel fuel module of a prismatic block VHTR. The results obtained from the coupled 3D and 1D models were in good agreement with that of a full 3D CFD analysis of the same specification and setup. However, the coupling strategy resulted in a stepwise constant profile for the axial variation in boundary values to be employed by Ansys Fluent for the coolant wall temperature. This stepwise profile was also reflected in the values obtained by the 1D/3D model for the variation in the temperature along the centreline of the fuel compact.

Within this study, the coupling methodology employed by Koekemoer *et al.* (2019) has been modified and automated to transfer a smoother profile for the coolant wall temperatures to be used as boundary conditions in Ansys Fluent. The models likewise consider 1/6th of the cross-section of the SCFM investigated by Travis & El-Genk (2013b). The Travis & El-Genk convection heat transfer correlation was employed to couple the heat transfer between the 1D and 3D formulations. The validity of the 1D/3D co-simulation methodology was investigated by comparing the temperature distribution in a single-channel fuel module for an (i) uniform- and (ii) cosine power profile with the corresponding values obtained from an explicit 3D model of the fuel compacts, graphite moderator and coolant channel of 1/6th of the SCFM model created in STAR-CCM+.

2. Single-Channel Fuel Module

As a typical prismatic VHTR, the PMR600 is used as a reference reactor for the study. Fig. 1 shows a cross-sectional view of the reactor system of a PMR600. The active core consists of a series of hexagonal graphite fuel blocks stacked together to form columns. Cold helium enters the reactor system from the bottom and flows upwards to the upper plenum. The helium is collected within the upper plenum and flows downward into the core, cooling the fuel blocks before exiting through the lower plenum. The inner core section of the prismatic VHTR consists of columns of fuel assemblies with graphite reflector blocks at the top and bottom ends of the fuel assemblies. The graphite reflectors are added to reduce the amount of neutron leakage out of the system. The geometry of a standard fuel assembly of PMR600 is shown in Fig. 2. A fuel block consists of 102 coolant holes and 210 holes for rod-shaped fuel compacts.

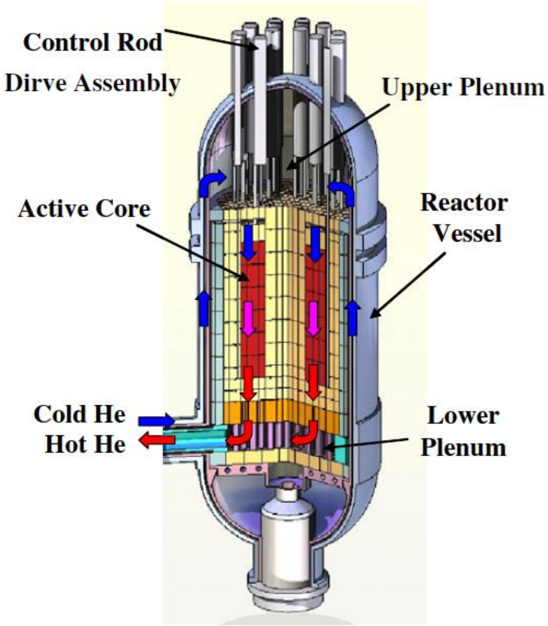


Figure 1: Reactor system of PMR600 and nominal flow sketch (Tak, *et al.*, 2008).

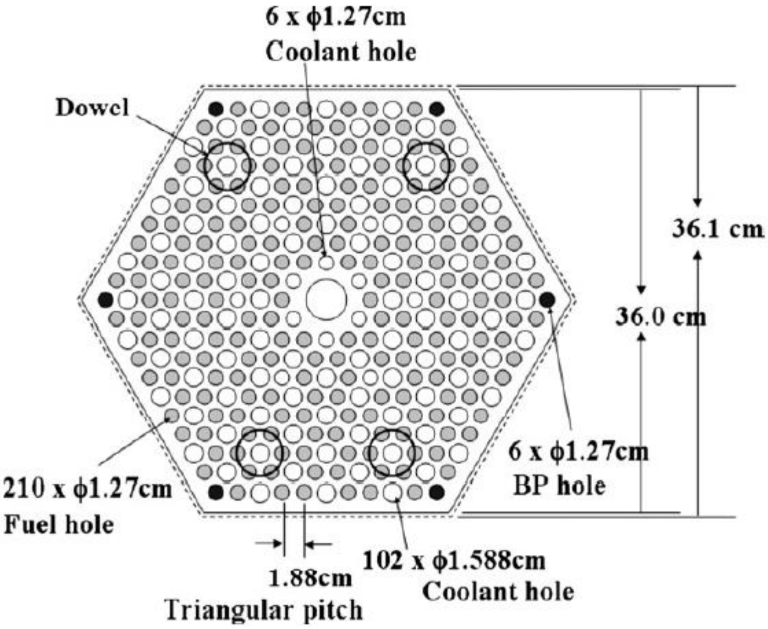
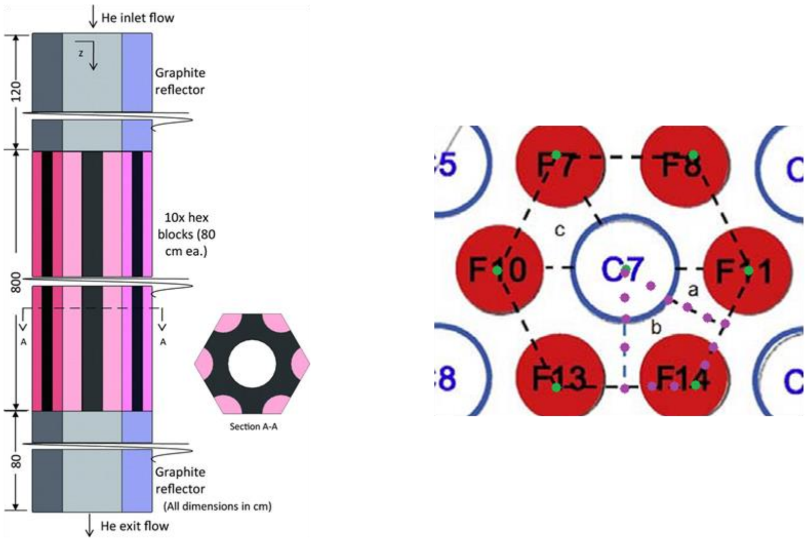


Figure 2: Top view of the standard fuel assembly of PMR600 (Tak, *et al.*, 2008)**.**

Within a fuel block, a single-channel fuel module consists of one coolant channel and six partial fuel compacts. Fig. 3(a) and Fig. 3(b) show an SCFM of a prismatic core block where the red elements in Fig. 3(b) represent the fuel compacts and the blue circle elements represent the coolant channels. Ten fuel blocks each with a height of 800 [mm] are stacked to form a fuel block assembly which has a total height of 8000 [mm]. The SCFM is represented by the hexagonal cross-sectional area contained around the coolant channel in Fig. 3(a) and the area outlined by the dashed hexagon in Fig.3(b). The fuel compacts have a diameter of 12.7 [mm] whereas the diameter of the coolant channels is 15.875 [mm] and the distance from a fuel compact center to the opposite fuel compact center is 37.6 [mm].



(a) (b)

Figure 3: (a) Side and top view of the SCFM (Travis & El-Genk, 2013b)**; and (b) dashed hexagon outline ng SCFM cross-section area** (Sambureni, 2015).

Based on the symmetry that can be observed in Fig. 3(b) only a section of the SCFM needs to be modelled. Three unit-cells that can be selected are indicated in Fig. 3(b) by the dashed areas *a*, *b*, and *c*. Unit cell *a* represents 1/12th of the SCFM, whilst unit cells *b* and *c* represent 1/6th of the single-channel fuel module. Unit cell *b* was selected for this study as Sambureni (2015) had already characterized and documented the conduction shape factors associated with the unit cell.

The inlet temperature, inlet pressure and mass flow rate of the helium-coolant were used as boundary conditions. The inlet- temperature and pressure of 914 [K] and 7.07 [MPa] respectively were assumed, with a mass flow rate of 0.0306 [kg/s] for the coolant. The total power applied to the SCFM was 55.4 [kW], which corresponds to a 600 [MW_{th}] HTGR (Travis & El-Genk, 2013b).

Two power profiles were assumed namely (i) a uniform distribution and (ii) a (chopped) cosine distribution. In the case of the uniform power distribution, a power density of 27.4026 [MW_{th}/m^3] was prescribed to correspond with the value used by Travis and El-Genk (2013b). For the cosine power profile the power density $PD(z)$ at a distance z from the entrance of the coolant channel is given as (Travis & El-Genk, 2013b) :

$$PD(z) = PD_{max} * \cos(0.2566 * z - 0.8831) \quad (1)$$

Where the maximum power density is given as PD_{max} = 33.135 [MW_{th}/m^3].

The properties of the different materials are given by the correlations summarized in Table 1.

Table 1: Material properties used in SCFM (Travis & El-Genk, 2013b)**.**

Property	Material	Correlation
Density, ρ (kg/m^3)	IG-110 graphite	1740
Specific heat, C_p (J/kg.K)		$6.05*10^{-7}T^3$ -0.00269T^2 +4.19T -294
Thermal conductivity, k (W/m.K)		-13.2 +2.50*10^4/$(T+268)^{0.78}$
Density, ρ (kg/m^3)	Composite Fuel	1650
Specific heat, C_p (J/kg.K)		$3.11*10^{-7}$ T^3 -0.00155 T^2 +2.73 T -82.4
Thermal conductivity, k (W/m.K)		8.5 +7.68*10^4/$(T+268)^{0.995}$
Density, ρ (kg/m^3)	Helium	P/R_gT
Specific heat, C_p (J/kg.K)		5197.6
Thermal conductivity, k (W/m.K)		0.000258 T +0.103388
Dynamic viscosity, μ (Pa-s)		0.03319 T +13.0744

Based on the result obtained by Travis and El-Genk (2013b) it was found that for the conditions given we have that $4.46\times10^4 < \mathrm{Re} < 5.65\times10^4$ and $1.28\times10^3 < Ra < 7.92\times10^3$. These result in an Aicher number of $Ai < 0.05$ and the convection heat transfer regime can therefore be considered as turbulent forced convection heat transfer as shown in Fig. 4.

3. Single-Channel Fuel Module Modelling and Validation

3.1 Travis and El-Genk

Travis and El-Genk (2013b) used the CFD code STAR-CCM+ to perform an explicit 3D detailed simulation of a SCFM to evaluate various convection heat transfer correlations. From the results obtained, the authors developed an improved turbulent convection heat transfer correlation and implemented it in a coupled 3D/1D simulation of a heat transfer and fluid flow associated with a SCFM. In the explicit 3D simulation prism layer meshes were used at the interfaces between the graphite moderator and the coolant channel as well as at the interface between the fuel compact and that of the graphite moderator. A grid dependence study was performed by Travis & El-Genk (2013b) and the final mesh that was employed in the simulations consisted of 6.67 million cells.

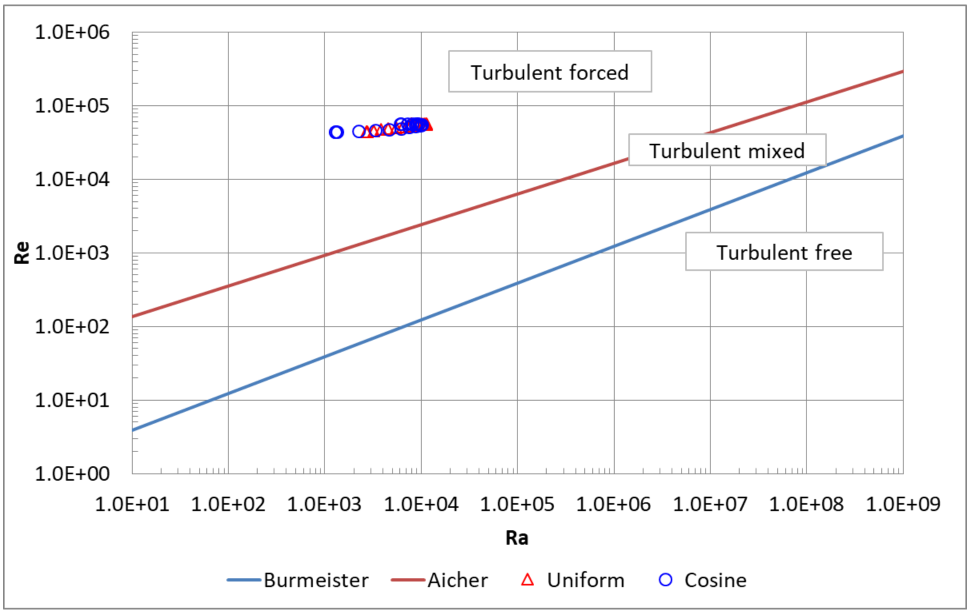


Figure 4: Convection heat transfer regime for SCFM

For Travis and El-Genk (2013b) to calculate the heat transfer coefficient, the bulk fluid temperature, T_b, the wall temperatures, T_w, as well as the heat fluxes at the wall surface of the coolant channel, had to be extracted from the explicit 3D simulations. The authors used the extracted data to calculate the convection heat transfer coefficient and formulate a new heat transfer correlation. They then implemented the proposed correlation into a coupled 3D/1D simulation using STAR-CCM+ to model the 3D heat transfer in the fuel compact and moderator graphite and a 1D approach for the fluid flow in the coolant channel.

Fig. 5 illustrates the comparison of the local heat transfer coefficient and the bulk fluid temperature obtained using coupled 3D/1D and 3D simulation of the SCFM (Travis & El-Genk, 2013b). It can be seen that both the heat transfer coefficient and bulk fluid temperature of the coupled 3D/1D and full 3D simulation are in good agreement with one another.

Travis and El-Genk (2013b) subsequently applied the 3D/1D methodology to simulate the heat transfer and flow in 1/6th of a full-height prismatic core and concluded that the results confirmed the effectiveness of the methodology.

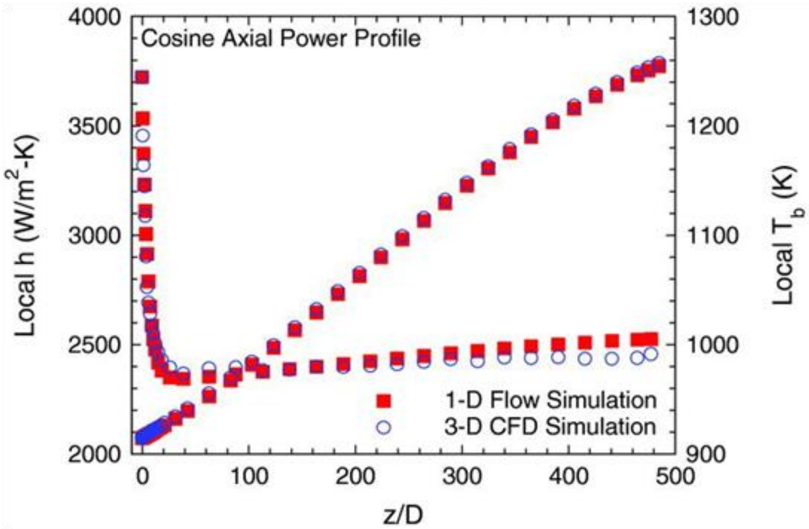


Figure 5: Comparison of the values of the local heat transfer coefficient and the bulk fluid temperature obtained using coupled 3D/1D and 3D simulations of the SCFM (Travis & El-Genk, 2013b).

3.2 3D STAR-CCM+ Model

To validate the coupled 1D/3D model used within this study, a full 3D model consisting of the fuel compact, graphite moderator and coolant channel of 1/6th of the SCFM was created using the CFD code STAR-CCM+. This explicit 3D model was constructed to recreate the results obtained by Travis and El-Genk (2013b) and aid in the investigation of the validity of the coupled 1D/3D methodology.

Using Solidworks (Dassault Systems, 2017), the geometry of the entire SCFM was constructed and assembled. The assembled section was 1200 [mm] long and consisted of the fuel compact, graphite moderator and coolant channel. The assembly was imported into STAR-CCM+ whereafter the necessary parts and surfaces were split and renamed as needed. Three different regions and material continua were created and assigned to the different parts and faces. Table 1 contains the material properties used within the material continua for the fuel rod, graphite moderator and helium before assigning it to the relevant region. A single mesh continuum was constructed in STAR-CCM+ to ensure that the faces on the interfaces between adjacent parts (Fuel rod, graphite moderator, and coolant channel) matched to form a conformal mesh. By using a single mesh continua no interpolation was necessary when transferring information across interfaces. This also aided in the stability of the solution. The base size for the mesh was chosen to be 6 [mm] similar to the mesh size employed by Travis and El-Genk (2013b). Five prism layers were used at the interfaces between the fuel compact and moderator graphite, and the interface between the moderator graphite and the coolant channel. The total thickness of the five prism layers was 0.4 [mm] with a layer stretching factor of 1.2. The use of the prism layers allowed for temperature gradients at the interfaces to be resolved sufficiently whilst also aiding in the overall stability of the solution. The prism layers, mesh, and conformal mapping across the interfaces for the generated STAR-CCM+ mesh can be seen in Fig 6.

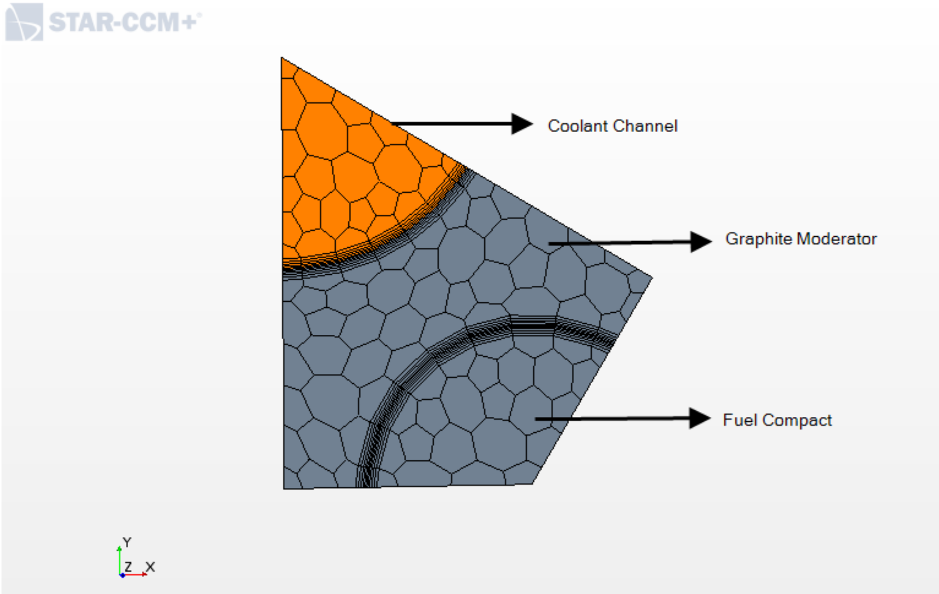


Figure 6: Cross-section of STAR-CCM+ mesh

Within the mesh continua, the polyhedral growth rate, density, and volume blending were set to 1, while a surface growth rate of 1.3 was added with a minimum size of 25% and maximum size of 100% of the base size of the mesh. The volume mesh for the 1200[mm] section of the SCFM could then be generated. The mesh was then used as the basis for the extrusion meshing scheme used within the simulations. The total length of the 1/6th SCFM required for the simulations was 9200 [mm] to account for the height of the 8000 [mm] heated section shown in Fig 3 (a) as well as the top reflector. Travis and El-Genk (2013b) commented that 75 coolant diameters (resulting in a 1200 [mm] length top reflector) would be sufficient for fully developed turbulent flow to occur at the entrance of the heated section. The mesh was extruded from the top faces of the fuel compact, moderator graphite and the coolant channel regions of the original 1200 [mm] section of the SCFM. The extrusion consisted of 11500 layers and was specified to be normal to the surfaces. The total length of the extruded mesh was set to 9200 [mm], which resulted in each layer having a thickness of 0.8 [mm]. The layer thickness was similar to the size of the axial increments used by Travis and El-Genk (2013b). Within this study, a mesh sensitivity study was deemed unnecessary as Travis and El-Genk (2013b) already performed a grid dependence study on the size of the mesh to be used for the 3D STAR-CCM+ model. Similar base size, meshing strategy and use of prism layers were employed to recreate the explicit 3D STAR-CCM+ model used by Travis and El-Genk (2013b).

After the extruded mesh was generated, the original volume mesh region was deleted from the simulation. New interfaces between the moderator graphite and coolant channel as well as between the fuel compact and moderator graphite had to be created. This approach ensured a uniform mesh distribution in the axial direction. The fuel compact region extended over the entire height (9200mm) of the SCFM model which resulted in the fuel compact properties also being assigned to the section in the reflector at the top of the model. This, however, had a negligible effect as no volumetric heat source was specified in this section.

Field functions were defined to specify the appropriate heat sources in the fuel compact region of the heated section to account for both the (i) uniform and (ii) cosine power profile.

Similar boundary conditions were applied to the full 3D CFD simulation as previously stated in Section 2. The calculated bulk fluid temperatures, wall temperatures, and the heat flux at the coolant channel wall were then used to obtain the local convection heat transfer coefficient. Fig 7 illustrates the bulk fluid temperatures and calculated heat transfer coefficient. These values were found to be in good agreement with the corresponding values predicted by the Travis and El-Genk correlation illustrated in Fig. 5. The wall temperature as a function of axial position for both a uniform- and cosine power profile is shown in Fig 8.

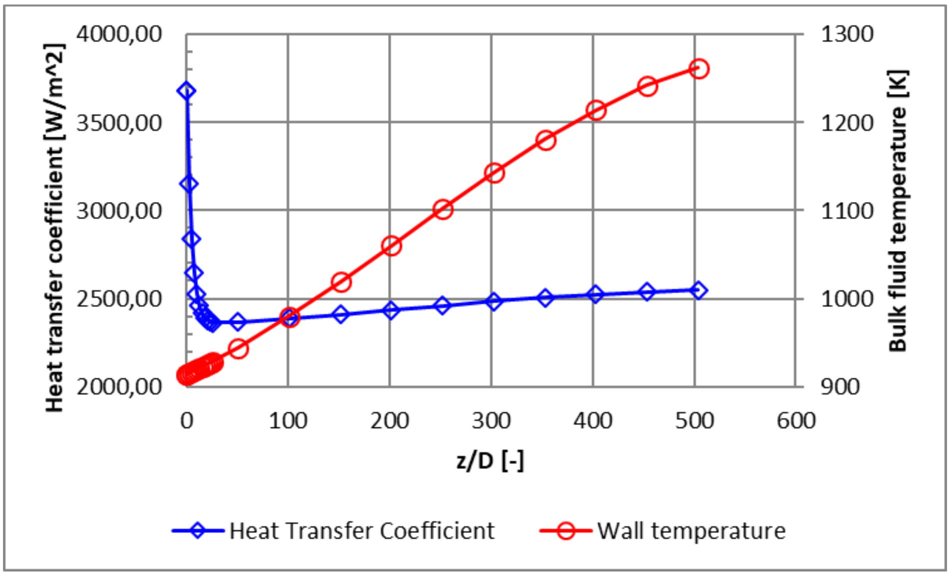


Figure 7: Heat transfer coefficient [W/m^2] and Bulk fluid temperature [K]

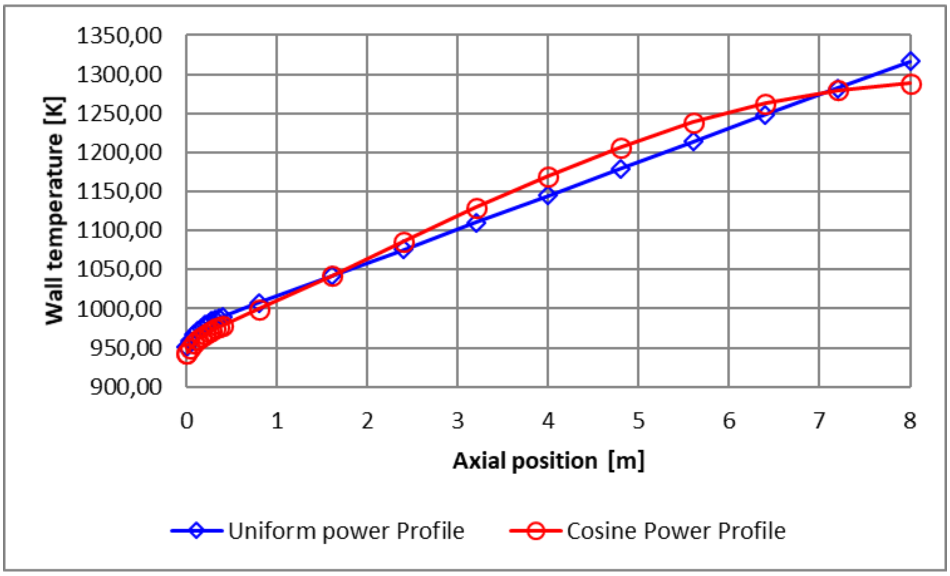


Figure 8: Wall Temperature as a function of axial position for a uniform and cosine power profile

4. 1D/3D Coupling methodology

Following Travis and El-Genk (2013b), 1/6th of the single-channel fuel module was also modelled using a coupled 1D/3D approach. The one-dimensional (1D) systems code, Flownex is used to simulate the fluid flow in the coolant channel whilst the 3D CFD code, Ansys Fluent, is employed to simulate the heat transfer in the fuel compact and graphite moderator. In general, both a 1D system- and a 3D CFD code are based on the conservation laws and empirical modes.

The principal path of heat transfer is formed where the heat is generated in the fuel compacts is conducted through the graphite block and is finally cooled down by convective heat transfer to the helium-coolant. The governing equation within the solid heat transfer is given as:

$$\frac{\partial}{\partial t}(\rho_s C p_s \mathrm{T_s}) + \Delta * (-\mathrm{k_s} \nabla \mathrm{T_s}) = \mathrm{q'''}_{\mathrm{gen}} \qquad (2)$$

For the fluid flow, Flownex solves the conservation equations which are simplified into 1D representations. These governing equations for flow in a pipe are given by Eq. 3-5 representing continuity, momentum, and energy respectively:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho V) = 0 \qquad (3)$$

$$\frac{\partial (\rho V)}{\partial t} + \frac{\partial (\rho V^2)}{\partial x} = -\frac{\partial p}{\partial x} - \rho g \frac{\partial z}{\partial x} - \frac{f \rho |V| V}{2D} \qquad (4)$$

$$\frac{\partial (\rho (h_o + gz) - p)}{\partial t} + \frac{\partial (\rho V (h_o + gz))}{\partial x} = \dot{Q}_h - \dot{W} \qquad (5)$$

During the normal operation of a very high-temperature gas-cooled reactor, the dominant mechanism of heat removal by the coolant can be considered to be convection. Therefore, in order to couple the heat transfer between solid and fluid, the convection heat transfer correlation needs to be implemented. Within this study, the correlation proposed by Travis and El-Genk (2013b) was implemented into both the coupled 1D/3D and full 3D STAR-CCM+ models. To account for developing flow ($z/D<25$) the adapted Travis and El-Genk (2013b) correlation given in Eq. (6) was used:

$$Nu = Nu_{FD} * (1 + 0.57 e^{-\frac{0.2z}{D}}) \qquad (6)$$

The correlation for the turbulent Nusselt number Nu_{FD} for fully developed flow for $z/D \geq 25$ is given as:

$$Nu_{FD} = 0.11 Re_b^{0.646} Pr_b^{0.4} \qquad (7)$$

with D the diameter of the coolant channel. Re_b and Pr_b are the Reynolds and Prandtl numbers based on the bulk temperature of the fluid.

Nel and Du Toit (2018) constructed a 1D model of 1/6th of a SCFM using the thermal-hydraulic systems code, Flownex. The model consisted of the fuel compact, graphite moderator, and coolant channel. The authors implemented the convection heat transfer coefficient correlation proposed by Travis and El-Genk (2013b) and found that the coolant channel wall temperatures were in good agreement with the corresponding temperatures obtained from Travis and El-Genk (2013b).

To simulate the heat transfer and fluid flow within the SCFM, the same number and size of increments used by Nel and Du Toit (2018) were implemented in both the 1D and 3D models.

4.1 1D simulation procedure

As Flownex accounts for the fluid flow within the coolant channel, the coupled 1D/3D CFD model only considers the 8000 [mm] heated section of the SCFM. The 75 coolant diameters (resulting in a 1200 [mm] length top reflector) is therefore not needed for the velocity profile to develop. The Flownex model is divided into forty-nine axial increments similar to the finest Flownex mesh used by Nel and Du Toit (2018). The first ten increments are each 40 [mm] long, followed by two 100 [mm] increments, and finally, thirty-seven increments that are each 200 [mm] in length. Fig. 9 illustrates the first two axial increments of the uncoupled Flownex model. In order to represent the flow and convection heat transfer in the coolant channel, the Flownex model only uses pipe and convection heat transfer elements.

The boundary conditions used for the Helium-coolant are listed in Table 2 and are the same as the corresponding boundary conditions used by Nel and Du Toit (2018) as well as the relevant boundary conditions used within the full 3D STAR-CCM+ simulations.

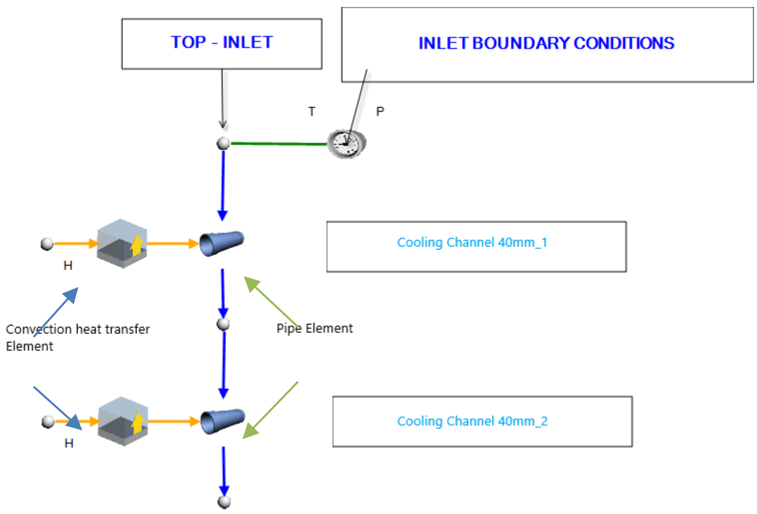


Figure 9: Inlet and first two increments of the coupled Flownex Model

Table 2: Inlet boundary conditions

Boundary Condition	Value
Inlet Temperature [K]	914 [K]
Inlet Pressure [MPa]	7.07 [MPa]
Mass Flow rate [kg/s]	0.0306 [kg/s]

4.2 3D simulation procedure

Similar to the 3D STAR-CCM+ modelling procedure, the 3D geometry of the single-channel fuel module consisting of the graphite moderator and fuel compact was created using Solidworks's CAD software. The 3D Ansys Fluent model was then divided into forty-nine axial increments corresponding to the axial increments implemented within the 1D Flownex model. After the geometry was imported into the Ansys Mesher, the different increments of the graphite moderator and fuel compact were categorized and assigned to reflect their nature, e.g. symmetry planes, interface, and walls. In the mesher, an inflation region was created on the moderator side of the coolant channel wall to propagate the prism layers from. Five prism layers were specified with a total thickness of 0.4 [mm], similar to that used within the 3D STAR-CCM+ model. A single mesh continuum using the tetrahedral meshing method was used for the entire model of the SCFM under investigation. The base size was selected to be 3 [mm]. To ensure no interpolation between adjacent parts and sub-assemblies were required a sweep and assembly meshing scheme was used to ensure a conformal mesh throughout the entire model. Fig. 10 (c) illustrates the conformal mapping across the interfaces and prism layers associated with the generated mesh. After the mesh was generated, the material properties and thermal conductivity correlations listed in Table 1 were implemented in Ansys Fluent. The different boundary conditions and input and output parameters (for data transfer from Flownex) were set and assigned. The power profiles for (i) uniform and (ii) cosine distribution were applied as heat flux sources on the two symmetry planes of the fuel compact. The version of Ansys Fluent used to perform the coupled 1D/3D simulations exhibited a problem when adding multiple volumetric heat sources, resulting in incorrect heat input to the system. To address this issue, the volumetric heat source data was transformed to heat flux data. This resulted in the correct amount of heat input to the system and was therfore implemented in both the (i) uniform and (ii) cosine power profile 1D/3D simulations.

4.3 1D/3D coupling procedure and solution algorithm

Flownex has a built-in link to Ansys Fluent (M-Tech Industrial, 2019b) allowing for scheme variables and parameters to be modified within Fluent's Text User Interface. By selecting Flownex as the managing or controlling code and to run Ansys Fluent in server/batch mode, Flownex and Ansys Fluent can be directly coupled. Using this methodology, users can solve 1D fluid flow and 3D heat transfer phenomena problems respectively by exchanging relevant data and information at interface boundaries (Ansys, 2021; M-Tech Industrial, 2019a). In the Flownex model, a server generic interface component was inserted to control the transfer of data and information between the different solvers. The server generic interface component as well as the data transfer links (dashed lines) that couple the Flownex wall nodes to the relevant Ansys Fluent input or output parameters can be seen in Fig. 10 (a) and Fig. 11.

The data transfer links account for the exchange of the coolant channel wall temperatures and the heat released by the coolant channel. Data transfer links must be defined for all forty-nine increments.

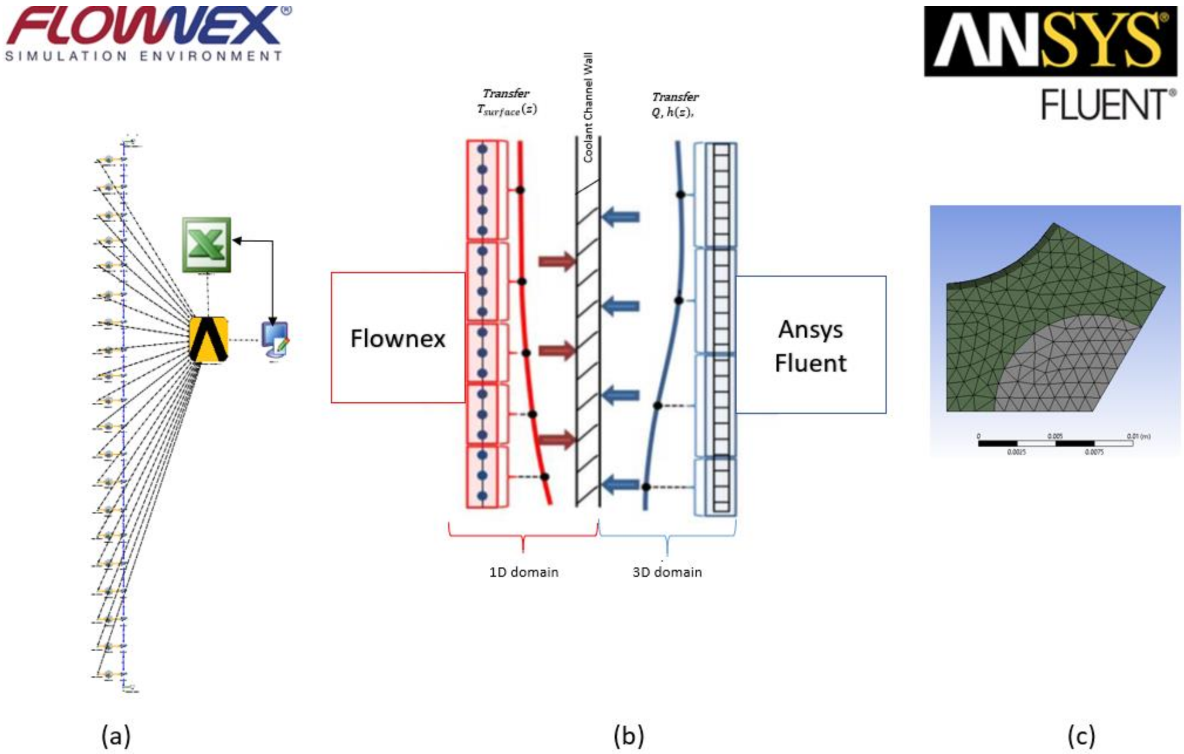


Figure 10: 1D/3D Coupling Process (a) Sample Flownex Network (b) Mapping procedure adapted from (Jordaan, et al., 2020) **(c) Cross-section of Ansys Fluent Mesh**

Koekemoer *et al* (2019) commented that the coupling strategy used to transfer data and relevant information between Flownex and Ansys Fluent should be investigated to determine whether a smoother profile for the coolant channel wall temperatures used as boundary conditions in Ansys Fluent could be established. This issue was addressed through the implementation of an Excel workbook and Scripting component within the Flownex model and can be seen in Fig. 10 (a). Typically in the coupled 3D/1D simulation used by Koekemoer *et al* (2019), Flownex calculates the average bulk fluid- and average coolant channel wall temperatures for each of the forty-nine increments. The schematic representation of the mapping procedure used in the 1D and 3D CFD domains can be seen in Fig. 10 (b). The blue dots embedded on the red line in Fig 10 (b) indicate the average coolant channel wall temperature as calculated by Flownex. Similarly, the black dots embedded on the blue line represent the heat flux/heat transfer rate for each increment being transferred from Ansys Fluent to Flownex. Jordaan, *et al.* (2020) concluded that this approach is only valid if the internal temperatures along the tubes are monotonically decreasing or increasing. This average coolant channel wall temperature ($T\_surface$) is then transferred from Flownex to Ansys Fluent for each of the forty-nine increments. Ansys Fluent uses these input parameters and applies the average surface temperature to the corresponding graphite moderator wall, resulting in a uniform temperature distribution throughout the entire increment. This strategy will result in a stepwise constant profile for the axial variation in boundary values to be employed by Ansys Fluent for the coolant wall temperatures.

This however is not optimal. Two methods exist to help smooth out the stepwise constant profile; (i) the total number of axial increments in both the Flownex and Ansys Fluent models can be increased, or (ii) User Defined Functions (UDFs) can be employed to transfer a more "representative" coolant channel wall temperature from Flownex to Ansys Fluent. This study opted for the use of UDFs to transfer the coolant channel wall temperature from the 1D domain to the 3D domain, as increasing the total number of axial increments is not a feasible option due to the time-consuming nature of model construction/set-up.

Fig. 11 illustrates an example mapping/interpolation of surface temperature for the first two, 40 [mm] long axial increments used within this study. Within the updated 1D/3D coupling procedure Flownex makes use of pipe- and convection heat transfer components, along with an excel workbook and scripting tool to calculate the average coolant channel wall temperature for each increment before transferring it to the excel workbook for processing. In the Excel workbook, the average coolant channel wall temperatures are converted to fitted polynomials. The coefficients associated with these polynomials are a function of the power profile (either (i) uniform, or (ii) cosine), the initial inlet temperature at the top of the increment, the average calculated coolant channel wall temperature, the length of the increment, and the total number of sub increment used. In Fig 11, the first two 40 [mm] increments are divided into 20 equally spaced sub increments, and the associated temperatures for each sub increment are shown. The surface temperature (UDF) being transferred to Ansys Fluent is in the form:

$$T\_surface\ (z) = f(PD(z), T\_Initial, T\_(surface, AVG), \Delta z, n\_subincrements) \qquad (8)$$

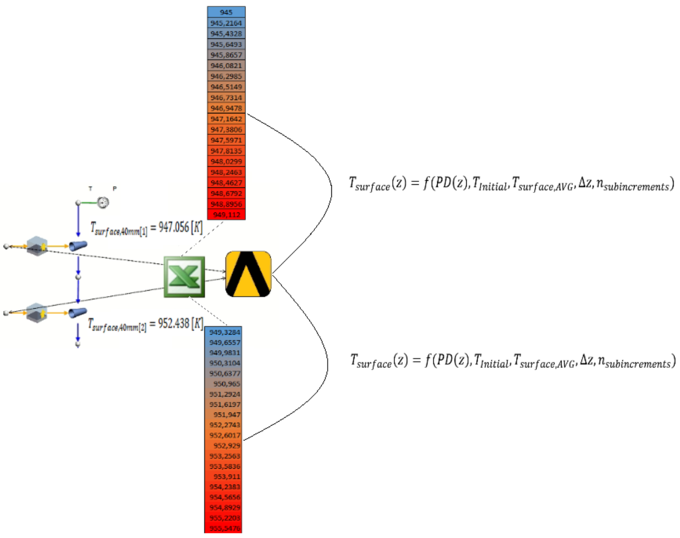


Figure 11: Example Mapping/Interpolation of Surface Temperature for the uniform power profile

This mapping procedure illustrated in Fig 10 (b) and Fig. 11 allows for automation and interpolation of node-averaged boundary conditions at the beginning and end of each increment to be established. Resulting in a smoother profile for the coolant wall temperature (depicted as a UDF) to be used as boundary conditions in Ansys Fluent. Successful co-simulation between Flownex and Ansys Fluent requires that principles of conservation at the interface between the 1D- and 3D domains be preserved. Semi-implicit or explicit coupling methodologies are available when coupling the thermal-hydraulic systems code Flownex to Ansys Fluent. The explicit coupling methodology was adopted for this study as data or relevant information is exchanged at regular intervals and the variables within the solvers are kept separate. Both interpolated node-averaged and boundary values were explicitly transferred between the two codes.

Fig. 12 depicts the solution algorithm employed for coupling Flownex and Ansys Fluent. Information transfer is initialized after steady-state conditions and interpolation of node-averaged boundary conditions within the Flownex model is achieved. Flownex then transfers the calculated surface temperature to Excel, in which a series of interpolation functions convert the average surface temperature into a UDF. The interpolated coolant channel wall temperature $T_{surface}$ in the form of a UDF is then transferred to Ansys Fluent. These variables vary along with the vertical distance of the coolant channel, z, as the power profile per increment as well as the length of the increment changes. Following the data transfer from Flownex-Excel to Ansys Fluent, the 3D CFD simulation is initialized. Ansys Fluent iterates through a specified number of iterations before transferring a heat flux and convective heat transfer coefficient h back to Flownex. After the information exchange between Flownex and Ansys Fluent the global iteration advances. This process is repeated until acceptable convergence criteria of $1e^{-04}$ for the Flownex solver and $1e^{-06}$ for Ansys Fluent is achieved.

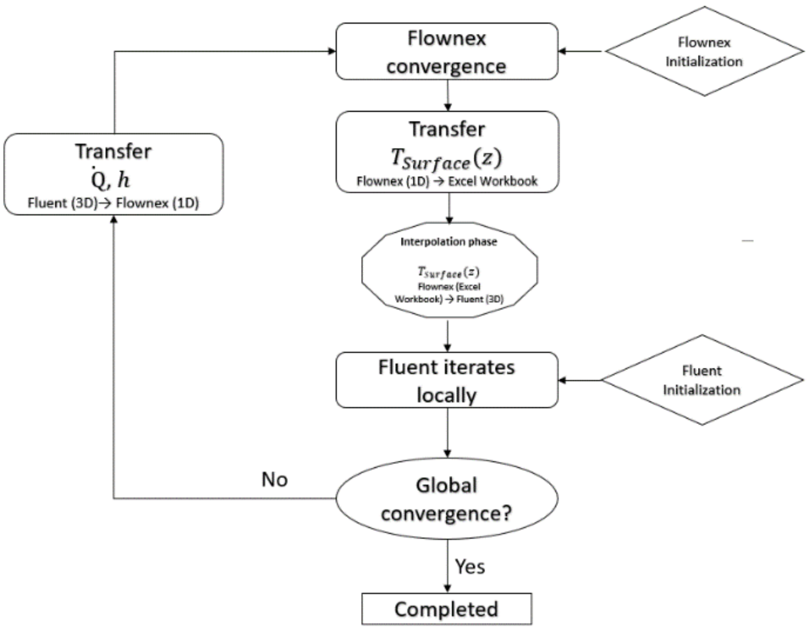


Figure 12: Solution Algorithm for coupling Flownex and Ansys Fluent

5. Results and Discussions

By comparing the temperature distributions in a single-channel fuel module for a (i) uniform and (ii) (chopped) cosine power profile with the equivalent values obtained from a full 3D CFD simulation of the same specification and set up, the validity of the coupled 1D/3D methodology is explored. Fig. 13 and Fig. 14 illustrate the radial temperature distribution generated by the full 3D STAR-CCM+ model, coupled 3D/1D model (Koekemoer, et al., 2019), and improved 1D/3D model at three distinct axial points within the SCFM. These axial locations are at $z/D = 25.1968$, $z/D = 151.181$, and $z/D = 302.3622$. The radial distributions run from the center of the coolant channel to the center of the fuel compact. The results obtained for the uniform power profile are shown in Fig. 13, while the results obtained for the cosine power profile are shown in Fig. 14.

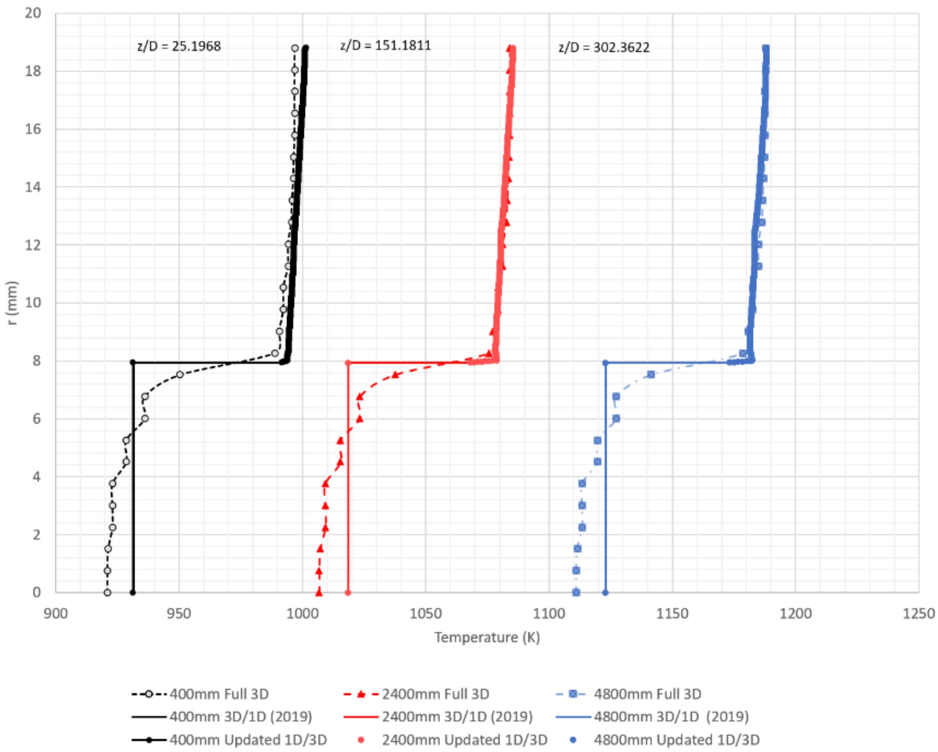


Figure 13: Radial temperature distribution at three axial locations for the 3D, 3D/1D and Updated 1D/3D uniform power profile

The agreement between the temperature changes predicted by the full 3D model and coupled 1D/3D model for the fuel compact and moderator graphite can be seen in both Fig. 13 and Fig. 14. On the graphs, the moderator graphite and fuel compact occur between 7.94 [mm] and 18.8 [mm]. The temperature variation predicted by the complete 3D model and the coupled 3D/1D model reflects the fact that the coupled 3D/1D model (2019) can only estimate the bulk fluid temperatures.

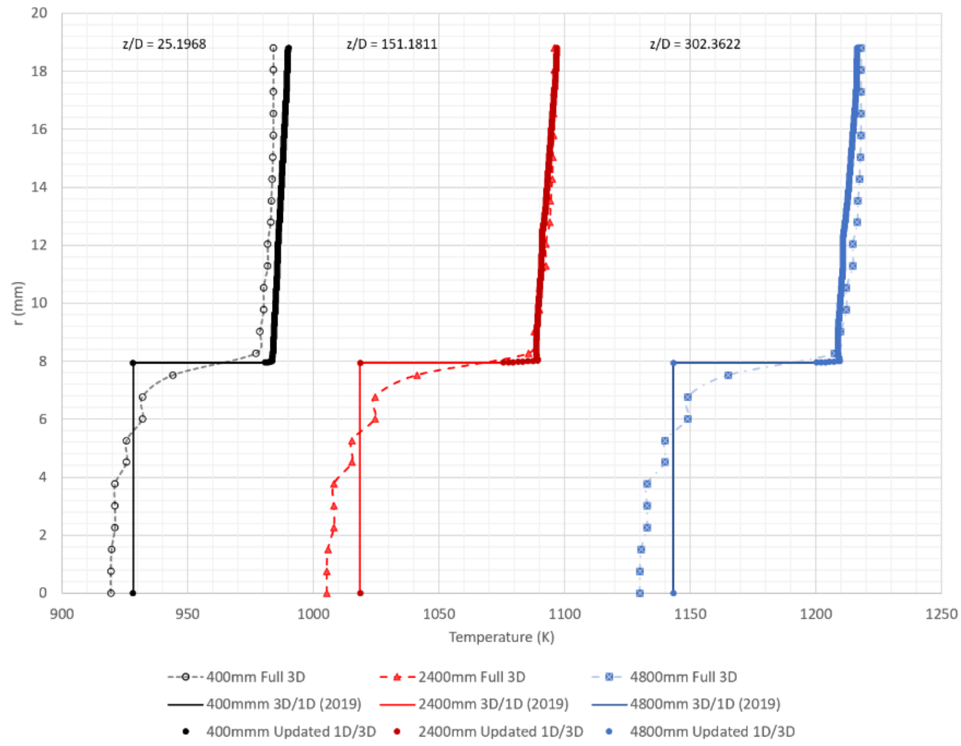


Figure 14: Radial temperature distribution at three axial locations for the 3D, 3D/1D and Updated 1D/3D Cosine power profile

In Fig. 15 and Fig 16, the axial variation in temperature at the center of the fuel compact for the uniform and cosine power profiles as produced in the coupled 1D/3D model is respectively compared to the full 3D STAR-CCM+ model's comparable results. It can be seen that the agreement for both the uniform- and cosine power profiles is very good. For the uniform power profile, a maximum deviation of 0.78 % can be observed, whilst for the cosine power profile the error percentage increase to 1.13 %.

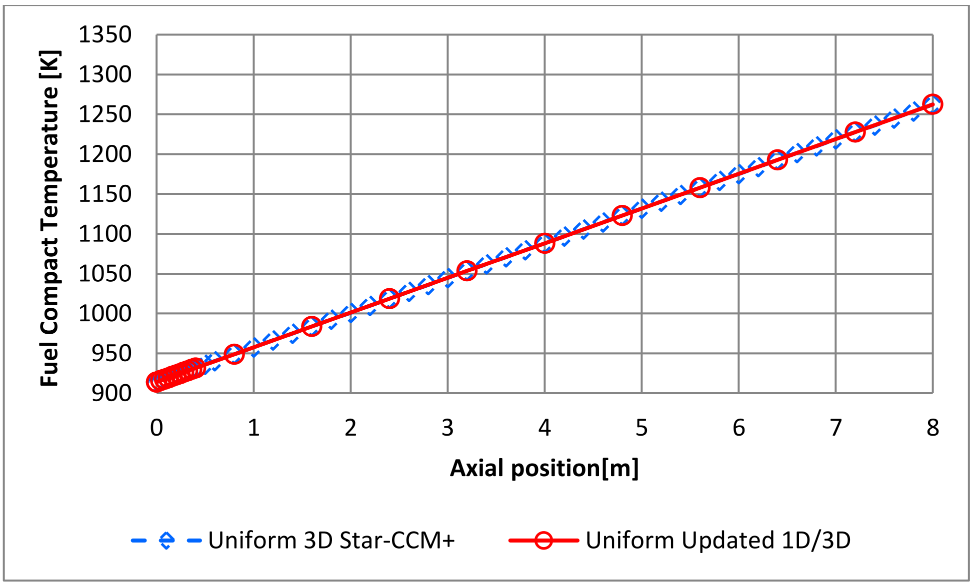


Figure 15: Fuel compact temperature as a function of axial position for the uniform power profile

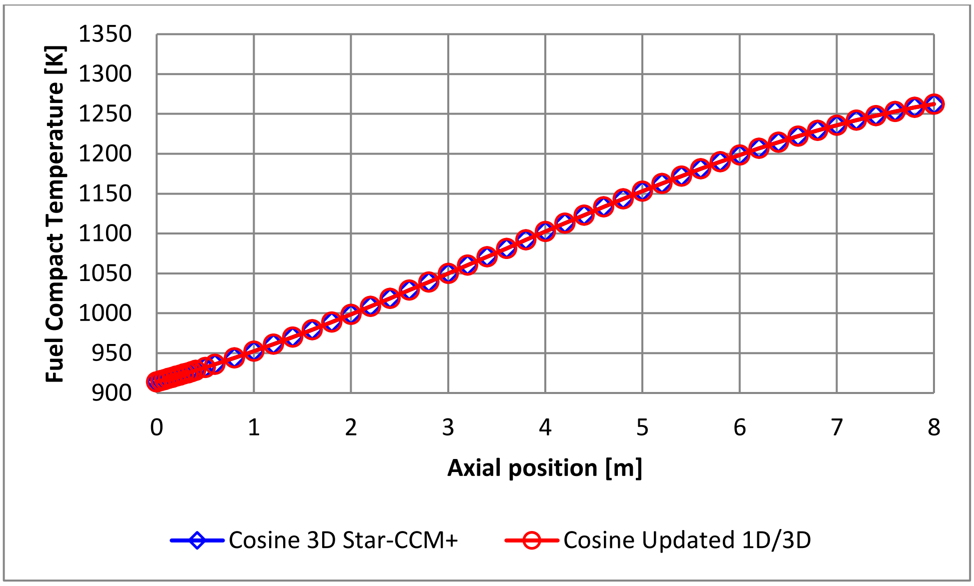


Figure 16: Fuel compact temperature as a function of axial position for the uniform power profile

Fig. 17 and Fig. 18 show the comparison between the results obtained by the coupled 1D/3D model and the full 3D STAR-CCM+ model for the variation in the axial direction of the coolant wall temperature for the uniform- and cosine power profile, respectively. It can again be seen that the agreement between the corresponding results is very good. The coupled 1D/3D models indicate errors between the calculated coolant channel wall temperatures for the uniform power profile to be 1.27 %, while for the cosine power profile the error increase to 1.46 %.

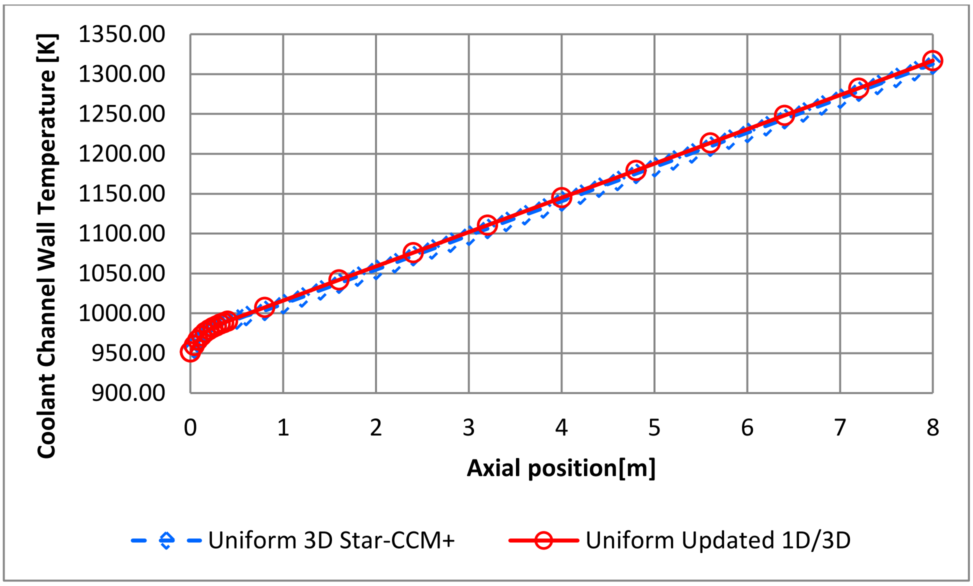


Figure 17: Coolant Channel wall temperature as a function of axial position for the uniform power profile

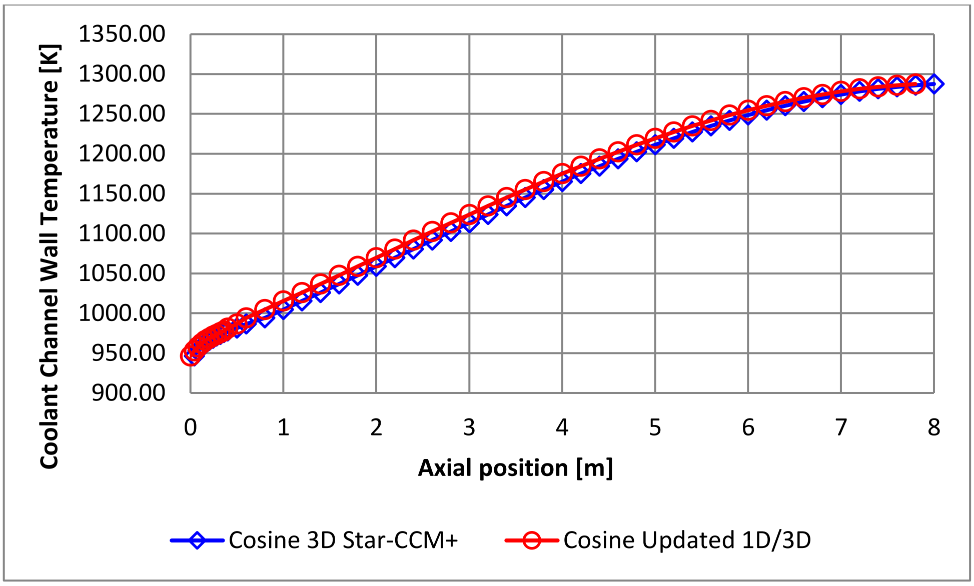


Figure 18: Coolant Channel wall temperature as a function of axial position for the uniform power profile

Table 3 illustrates the resource comparison between the explicit 3D CFD STAR-CCM+ model and the 1D/3D co-simulation. From the results gathered a model size reduction of 60 % can be observed. The coupled 1D/3D models indicate errors between the calculated fuel- and coolant temperatures for both a (i) uniform, and (ii) cosine power profile of less than 1.5%, when compared to a full CFD analysis of the same system. The 1D/3D co-simulation model also takes 1/5th of the time to reach a converged solution, when compared to the explicit 3D CFD model.

Table 3: Computational resource comparison

	1D/3D co-simulation	**Explicit 3D STAR-CCM+**
Number of cells [-]	1 175 585 [-]	2 967 000 [-]
Global iterations [-]	17 [-]	0 [-]
Time per iteration [s]	2.43 [s]	1.43 [s]
Number of iterations [-]	2 840	22 668 [-]
Data transfer time [s]	3 [s]	0 [s]
Solution time [s]	6 953 [s]	32 415 [s]

6. Summary and Conclusion

Simulating the thermal-hydraulic behaviour and predicting accurate nuclear fuel- and coolant temperatures in prismatic block reactor units poses several challenges and typically requires significant computational resources and computational times. This paper discussed an updated coupled 1D/3D simulation methodology used to simulate the fluid flow and heat transfer in a single-channel fuel module of a prismatic fuel block. By coupling the one-dimensional (1D) systems code Flownex and the three-dimensional (3D) CFD code Ansys Fluent the strengths of each respective code were leveraged. Flownex was used to simulate the fluid flow in the coolant channel whilst the heat transfer in the fuel compact and graphite moderator was modelled using Ansys Fluent. The study performed by Travis and El-Genk (2013b) served as a basis for the current study.

Within this study, the stepwise constant profile for the axial variation in boundary values transferred between Flownex and Ansys Fluent as identified by Koekemoer *et al.* (2019) was addressed. An explicit 3D model consisting of the fuel compact, graphite moderator and coolant channel of 1/6th of the SCFM was created using the CFD code STAR-CCM+ to assist in the validation of the proposed coupled 1D/3D methodology.

By comparing the temperature distribution in the single-channel fuel model for a (i) uniform- and (ii) cosine power profile with the corresponding values obtained from published work, as well as a full detailed 3D CFD analysis of the same specifications and setup, the validity of the coupled 3D/1D model was investigated. Due to the symmetry present in the single-channel fuel module, the models developed in the study considered only 1/6th of the cross-section of the SCFM. The proposed Travis and El-Genk (2013b) correlation was implemented into both the coupled 1D/3D and full 3D STAR-CCM+ models. The coupled 1D/3D models indicated errors between the calculated fuel- and coolant temperatures for both an (i) uniform, and (ii) cosine power profile of less than 1.5%, when compared to a full CFD analysis of the same system. By explicitly coupling the 1D and 3D solvers the computational expense was greatly reduced when compared to full CFD. Therefore, the coupled 1D/3D methodology can form the basis of an integrated model for the entire prismatic core.

CRediT authorship contribution statement

O.C. Koekemoer: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation, Formal analysis, Writing – Original Draft, Project administration.

Prof. C.G. du Toit: Conceptualization, Supervision, Writing – review and editing. Project administration.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Any opinion, finding and conclusion or recommendation expressed in this material is that of the author(s) and the NRF does not accept any liability in this regard.

Nomenclature

Abbreviations

1D	One-dimensional
3D	Three-dimensional
CFD	Computational Fluid Dynamics
HTGR	High Temperature Gas Reactor
HTTR	High Temperature Test Reactor
HTR	High Temperature Reactor
NPP	Nuclear Power Plant
SCFM	Single-Channel Fuel Module
TRISO	Tristructural-isotropic
UDF	User defined function
VHTR	Very High Temperature gas-cooled Reactor

Symbols

C_p	Specific heat [J/kg-K]
D	Diameter [m]
k	Thermal conductivity [W/m-K]

μ	Dynamic viscosity [Pa-s]
Nu	Nusselt Number
P	Pressure
Pr	Prandtl Number
R_g	Universal gas constant
Re	Reynolds Number
ρ	Density [kg/m^3]
T	Temperature [K]
z	Cartesian axis direction [m]

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5. SUMMARY AND CONCLUSIONS

Co-simulation has been applied in various domains and scenarios, often without a comprehensive study on the impact to simulation- stability, time, and results. The purpose of this study was to investigate several 1D/3D co-simulation methodologies as applied to High Temperature Reactors (HTRs) and subsystems. The development and validation of different co-simulation strategies that couple the thermal-hydraulic systems code, Flownex with the three-dimensional (3D) Computational Fluid Dynamics (CFD) code, Ansys Fluent was investigated.

Understanding the thermal behaviour and predicting accurate fuel- and coolant temperatures are of considerable importance in the design of Very High Temperature gas-cooled Reactors (VHTRs). However, the modelling of prismatic block high-temperature gas-cooled reactor units pose several challenges and typically requires significant computational resources and computational times. By employing a coupled 1D/3D methodology, the desired features of a one-dimensional (1D) systems code and a three-dimensional (3D) Computational Fluid Dynamics (CFD) code can be leveraged to help reduce the CFD computational expense whilst still retaining an acceptable level of accuracy. This was achieved by demonstrating a coupled 1D/3D CFD model that simulates the heat transfer and fluid flow in a single-channel fuel module of a prismatic block. The coupled 1D/3D model represented $1/6^{th}$ of a single-channel fuel model that accounts for conduction heat transfer in the solids, convection heat transfer between the solids and the fluid and the fluid flow in the coolant channel. To validate the coupled 1D/3D SCFM model utilized in this study, an explicit 3D STAR-CCM+ CFD model of the SCFM was constructed. The results for the coolant channel wall temperatures and fuel compact centre temperatures were found to be in very good agreement with corresponding values predicted by the full 3D explicit model.

Four different 1D/3D co-simulation methodologies were explored to investigate the radiative- and convective- heat transfer, and natural circulation phenomena occurring in a simplified water-cooled RCCS facility. All four 1D/3D co-simulation methodologies' associated temperatures, mass flow rates, and riser power were found to be in good agreement with the validated full one-dimensional (1D) simulation results. By investigation of the different 1D/3D co-simulation methodologies the impact on simulation- stability, -time, and results were investigated to help serve as a basis for future 1D/3D co-simulation implementations.

The preferred 1D/3D co-simulation methodology was found to be the directly coupled-parallel approach. Within this strategy, a temperature and a heat flux/heat transfer rate are being transferred between the different codes/solvers in an explicit manner. This approach is robust, requires less computational resources and reaches a converged solution in the least number of iterations and amount of solution time.

Using the directly coupled-parallel approach the heat transfer in a prismatic block VHTR was simulated using a coupled 1D/3D methodology. It is worth noting that even though the same SCFM was simulated, the solution strategy and the methodology used to transfer data between Flownex and Ansys Fluent was different. Also, previously defined shortcomings were addressed. The work performed was inspired by Travis and El-Genk (2013b) and Nel and Du Toit (2018). Validation of the coupled 1D/3D methodology was done using corresponding values obtained from published work (Travis and El-Genk, 2013b) and full explicit 3D CFD. When compared to an explicit 3D CFD analysis of the same system, the coupled 1D/3D projections suggest errors between the calculated fuel- and coolant temperatures of less than 1.5% for both a (i) uniform, and (ii) cosine power profile. When compared to explicit 3D CFD, a model size reduction of 60 % can be observed. The 1D/3D co-simulation model also takes 1/5th of the time to reach a converged solution, when compared to the explicit 3D CFD model.

It is recommended that any of the 1D/3D co-simulation methodologies investigated within this study may be implemented for the thermal-hydraulic analysis of HTRs and accompanying systems.

1D AND 3D CFD MODELS OF THE HEAT TRANSFER IN A PRISMATIC BLOCK OF A VHTR

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ABSTRACT

The VHTR (Very High Temperature Reactor) prismatic block reactor is one of the reactor designs considered in the range of 4th Generation Reactors which are under development today. The heat generated by the gas-cooled reactor can be used to produce electricity or as process heat to produce amongst others hydrogen. For the operation of the reactor under normal and upset conditions the conduction heat transfer through the prismatic block and the convection heat transfer to coolant is of critical importance. This paper discusses 3D and 1D computational fluid dynamic (CFD) models to simulate the heat transfer and fluid flow in a single-channel fuel module of a prismatic block. These models account for conduction heat transfer in the solids, convection heat transfer between the solids and fluid and fluid flow in the coolant channel in the single-channel fuel module. The current models represent one sixth of a single-channel fuel module. Detailed results are obtained for uniform and cosine power profiles by employing a 3D CFD code whilst representative results are obtained by a 1D system CFD code. The models are evaluated by comparing the temperature distribution results of the fuel compacts, coolant channel wall and the coolant, obtained by the different models with each other. The analyses of the study are performed employing the 3D CFD code STAR CCM+ and the 1D system CFD code Flownex. The 1D model requires much less computational resources than the detail 3D CFD and can form the basis of an integrated model for the entire core.

1. Introduction

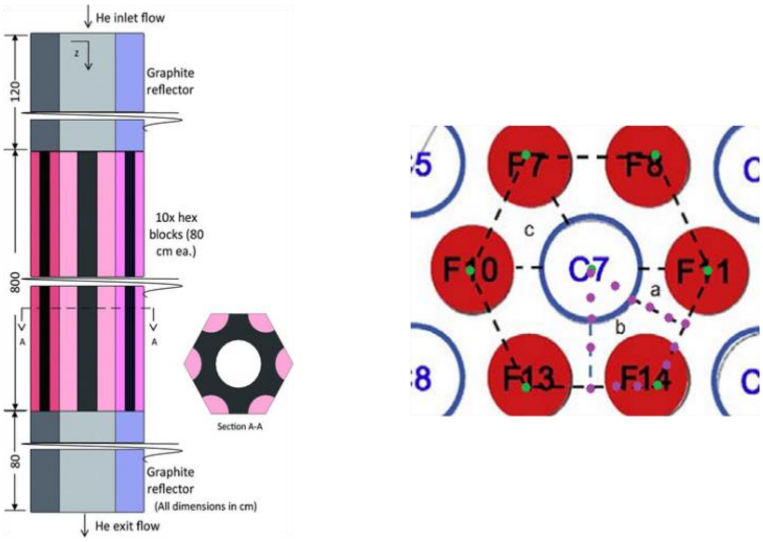
Generation IV nuclear reactor designs include the design for the Very High Temperature Reactor which has a thermal power output of 200–600 MWth. The reactors operate at outlet temperatures of 700 ˚C to 1000 ˚C and at a pressure of 4 MPa to 9 MPa (Travis & El-Genk, 2013b). Graphite is used for the moderator material and helium is used as the reactor coolant. The fuel compacts consist of Tristructural-isotropic (TRISO) particles dispersed in a graphite matrix. In the gas turbine- modular helium reactor (GT-MHR) prismatic fuel blocks are stacked to make 8000 mm fuel assemblies. A top graphite reflector of 1200 mm and a bottom graphite reflector of 800 mm are added to make the total fuel core height 10000 mm (Travis & El-Genk, 2013b).

The heat transfer and flow through the prismatic fuel blocks are very important for the safe operation of the VHTR core. Computational Fluid Dynamics (CFD) has been used in the industry to simulate different phenomena in the fuel blocks to a very accurate level. Johnson *et al*. (2012), Tak *et al.* (2008), and Tung *et al.* (2013; 2016) modelled 1/12th of a fuel assembly with explicit detail of the fuel compacts, graphite, coolant channels and bypass gaps. They studied the effect of prescribed power profiles and bypass gap size on the thermal-flow behaviour of the fuel assemblies. Tung *et al.* (2013; 2016) also studied the natural circulation that occurs after a loss of flow accident (LOFA). Johnson *et al.* (2012) used the CFD code ANSYS Fluent, Tak *et al*. (2008) the CFD code CFX, whilst Tung *et al*. (2013; 2016) used the CFD code STAR CCM+ (Siemens STAR-CCM+, 2018).

A convection heat transfer correlation was developed by Travis & El-Genk (2013b) to calculate the convection heat transfer coefficient for the helium in the coolant channels. In this study, the heat transfer and fluid flow were simulated in a representative manner using different CFD codes. The simulations used full 1D and full 3D CFD models to model a 1/6th Single Channel Fuel Module (SCFM). The 1D simulations are performed using Flownex and the full 3D simulations are executed by employing STAR CCM+. The simulations account for the conduction heat transfer through the fuel compact and moderator graphite, the convection heat transfer from the coolant channel wall to the coolant channel fluid and the flow of the coolant in the coolant channel. With the heat transfer through the SCFM accounted for the temperature distribution at the center and the wall of the fuel compact will be examined.

2. Single-channel fuel module

Within a fuel block a single channel fuel module consists of one coolant channel and six partial fuel compacts. Fig. 1(a) and (b) show a SCFM of a prismatic core block where the red elements in Fig. 1(b) represent the fuel compacts and the blue circle elements represent the coolant channels. Ten fuel blocks each with a height of 800 mm are stacked to form a fuel block assembly which has a total height of 8000 mm. The SCFM is represented by the hexagonal cross-sectional area contained around the coolant channel in Fig. 1(a) and the area outlined by the dashed hexagon in Fig. 1(b). The diameters of the fuel compacts and the coolant channels are respectively 12.7 mm and 15.875 mm and the distance from a fuel compact center to the adjacent fuel compact centre is 37.6 mm.



(a) (b)

Figure 1: (a) Side and top view of the SCFM (Travis & El-Genk, 2013b)**; and (b) dashed hexagon outlining SCFM cross sectional area** (Sambureni, 2015)

The temperature distribution, heat flux and flow through the coolant channel of the SCFM was studied by Travis and El-Genk (2013b) using a 3D CFD approach.

In Fig. 1(a) the different unit cells, namely *a, b* and *c,* that can be selected are shown. In this study unit cell *b* has been chosen as the most suitable and also because Sambureni (2015) has characterised the conduction shape factors required for a 1D analysis. This leads to the representing 1/6th of a SCFM.

The mass flow rate, inlet pressure and inlet temperature were used as boundary conditions. The mass flow rate was assumed to be 0.0306 kg/s and the inlet pressure to be 7.07 MPa, whilst the inlet temperature was assumed to be 914 K. The required material properties that are used is stated in Table 1. The total power applied to the SCFM was 55.4 kW which corresponds to a 600 MWth HTGR. Two power profiles were assumed namely a uniform distribution and a (chopped) cosine distribution. In the case of the uniform distribution a power density of 27.4026 MWth/m^3 was prescribed (Travis & El-Genk, 2013b). In case of the cosine power profile the power density PD(z) at the distance z from the entrance of the coolant channel is given as:

PD(z)=PD_max*cos (0.2566*z-0.8831) (Travis & El-Genk, 2013b)

Where the maximum power density is given as PD_max = 33.135 MWth/m^3.

Table 1. Properties of materials used in SCFM of a VHTR (Travis & El-Genk, 2013b)

Property	Material	Correlation
Density, ρ (kg/m^3)	IG-110 graphite	1740
Specific heat, C_p (J/kg.K)		$6.05*10^{-7}T^3$ -0.00269T^2 +4.19T -294
Thermal conductivity, k (W/m.K)		-13.2 +2.50*10^4/$(T+268)^{0.78}$
Density, ρ (kg/m^3)	Composite Fuel	1650
Specific heat, C_p (J/kg.K)		$3.11*10^{-7}$ T^3 -0.00155 T^2 +2.73 T -82.4
Thermal conductivity, k (W/m.K)		8.5 +7.68*10^4/$(T+268)^{0.995}$
Density, ρ (kg/m^3)	Helium	P/R_gT
Specific heat, C_p (J/kg.K)		5197.6
Thermal conductivity, k (W/m.K)		0.000258 T +0.103388
Dynamic viscosity, μ (Pa-s)		0.03319 T +13.0744

3. 1D Flownex

Flownex is a system-level simulation tool for the modelling of thermal-fluid systems and is used in many industries in the design and optimization of thermal-fluid systems. Flownex calculates amongst others the flow rates, temperatures, pressures and heat transfer rates using both steady-state and transient models (M-Tech Industrial, 2017).

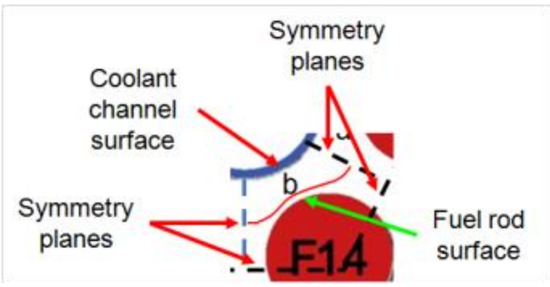


Figure 2: Unit cell for conduction between fuel compact and coolant channel.

In Fig.2 only a 1/6th of a SCFM is shown and will be modelled in Flownex due to the geometry symmetry as stated previously. With the symmetry model used in Flownex, the model will consist out of 1/6th of a coolant channel, the accompanying graphite matrix and a 1/3rd of a fuel compact. The basic setup of the Flownex model of the SCFM is described in Fig. 3. The conduction through the fuel compact is represented by a single conduction element and the conduction through the graphite moderator is represented by two conduction elements. For the conduction through the moderator, represented by the two conduction elements, the conduction lengths and areas needed were calculated by Sambureni (2015). The coolant channel section is characterized by the use of a convection element and a pipe element to represent heat transfer from the coolant channel wall to the coolant fluid, as well as the advective heat transport in the coolant channel. The heat transfer coefficients used in the convection elements were obtained by employing the Nusselt number correlation derived by Travis & El-Genk (2013b).

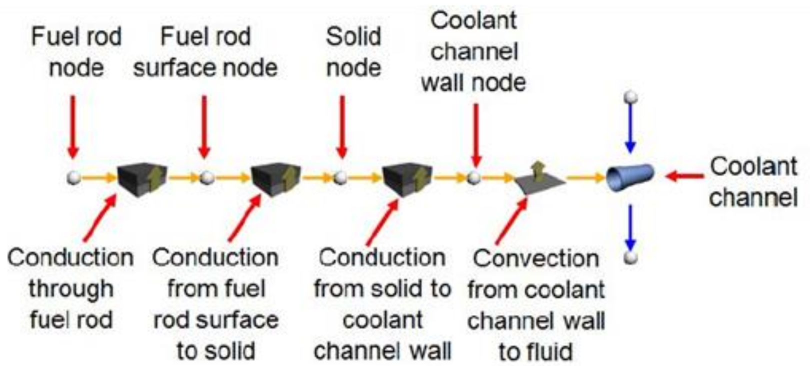


Figure 3: Flownex network for heat transfer from fuel rod and coolant channel

With the work performed by Nel & Du Toit (2018), the SCFM was discretized into 10 primary increments with each having a length of $\Delta z = 0.8$ m. As the inlet effects needs to be accounted for the first increment is divided into ten 0.04 m and one 0.4 m increments respectively which leads to 20 increment layers in total.

As it can be seen in Fig. 4 a model is shown that represents the ten primary increments used to model the SCFM. With the current study, two additional models were constructed where the increment count was increased to 30 and 49. The increased increment count accounts for the increments between 0.4 m and 8 m. Thus, the coarse grid consists of 20 increments, the medium grid of 30 increments and the fine grid of 49 increments. In all three models, the effect of the uniform and cosine power profiles were considered.

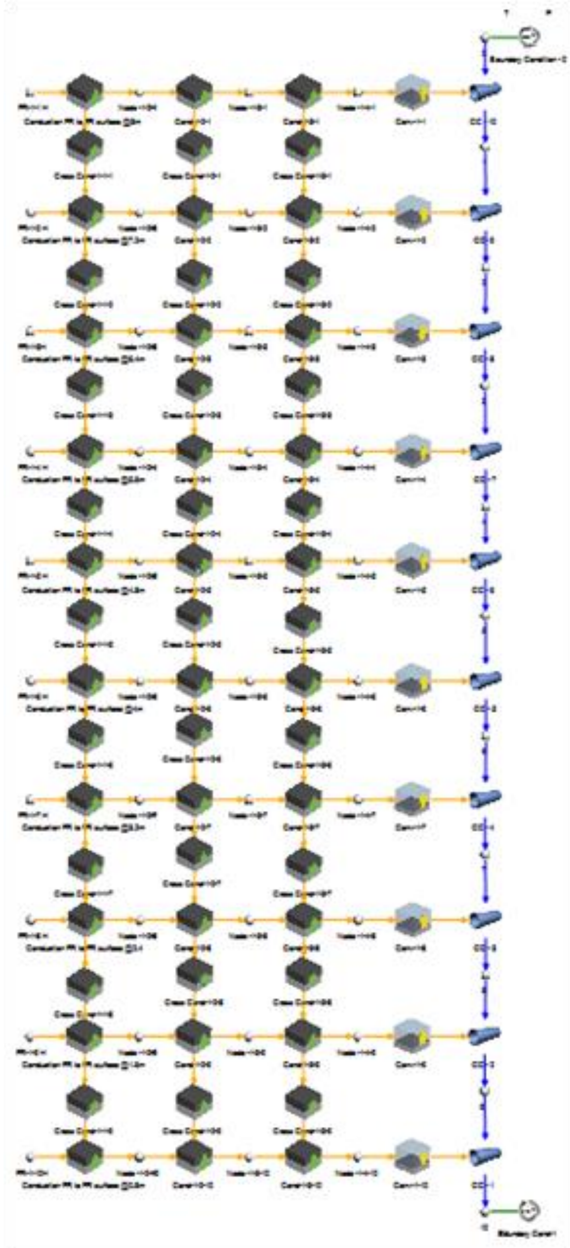


Figure 4: 800 mm x 10 increment Flownex model

4. 3D STAR CCM+

With the 1D model of the SCFM constructed and simulated in Flownex a full 3D model of the SCFM was simulated in STAR CCM+ (Siemens STAR-CCM+, 2018) to evaluate the results obtained by the 1D simulations. The geometry of the SCFM model were constructed in Solidworks 2016 and imported into STAR CCM+ where the necessary regions and material continua were assigned. As three different materials were used, each material's continua properties were assigned as stated in Table 1.

A single mesh continuum was constructed for all the components in the model to ensure that the cells faces on the interface between adjacent parts matched to form a conformal mesh. This ensured that no interpolation was necessary for the transfer of information across interfaces. It was found to play an important role in the stability of the solution. A basic base size of 6 mm, based on the radius of the fuel compact, was chosen for the mesh. A number of five prism layers was selected and the layer thickness of all the layers was chosen such that each layer stretched by a factor of 1.2 and the total thickness of the five prism layers together was 0.4 mm. This ensured that the temperature gradients at the interfaces were resolved sufficiently and also assisted with the stability of the solution. The prism layers at the interfaces between the fuel compact and the moderator graphite, and those between the moderator graphite and the coolant channel can be seen in Fig. 5. The conformal mapping across the interfaces can also be seen.

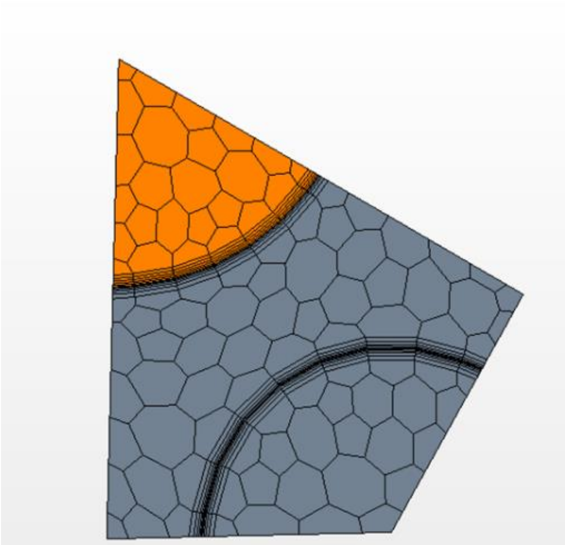


Figure 5: Cross section of STAR CCM+ (Full 3D) mesh.

The total length of the 1/6th SCFM model required for the simulations is 9200 mm to account for the top reflector and the height of 8000 mm of the heated section as shown in Fig. 1(a). Travis & El-Genk (2013b) commented that the 1200 mm length of the reflector is 75 coolant channel diameters which is sufficient for fully developed turbulent flow to occur at the entrance to the heated section.

An extruded mesh was implemented for the $1/6^{th}$ of the SCFM in the full 3D model. The models constructed accounts for three different layer heights for the extrusion that accounts for 1200 mm reflector and the 8000 mm heated section. In the work done by Nel & du Toit (2018), 11500 layers were extruded with a layer height of 0.8 mm which gives the required 9.2 m of the SCFM. In addition to the 0.8 mm, layer height extrusion model two additional layer height extrusion models of which the heights are 1.6 mm and 0.4 mm were considered. The additional models with the different layer heights add up to 5750 and 23000 layers respectively that accounts for the 9200mm height of the $1/6^{th}$ SCFM. Thus, the coarse grid represents 5750 layers, the medium grid 11500 layers and the fine grid represents 23000 layers.

At the top of the coolant channel an inlet temperature of 914 K was specified, whilst an outlet pressure of 7.022 MPa was prescribed at the bottom of the coolant channel. The simulation was initialized by specifying a velocity inlet boundary condition of 41.5114 m/s which corresponded to the specified mass flow rate of 0.0051 kg/s. This helped to stabilize the solution during the initial phase of the simulation. Once the solution has stabilized the velocity boundary condition was replaced with the specified mass flow rate condition. The outside surfaces of the fuel compact and the moderator graphite were specified to be adiabatic and the outside surfaces of the coolant channel as symmetry planes.

5. Results

In the 1D Flownex models, the pressure and temperature at the inlet boundary were specified as 7.07 MPa and 914 K respectively. The outlet boundary condition is specified as a mass flow of which the flow rate is 0.0051 kg/s. As for the full 3D STAR CCM+ models the exact same inlet and outlet boundary conditions was used as in the full 1D models. The required results were extracted from the different Flownex and STAR CCM+ models and compared with each other.

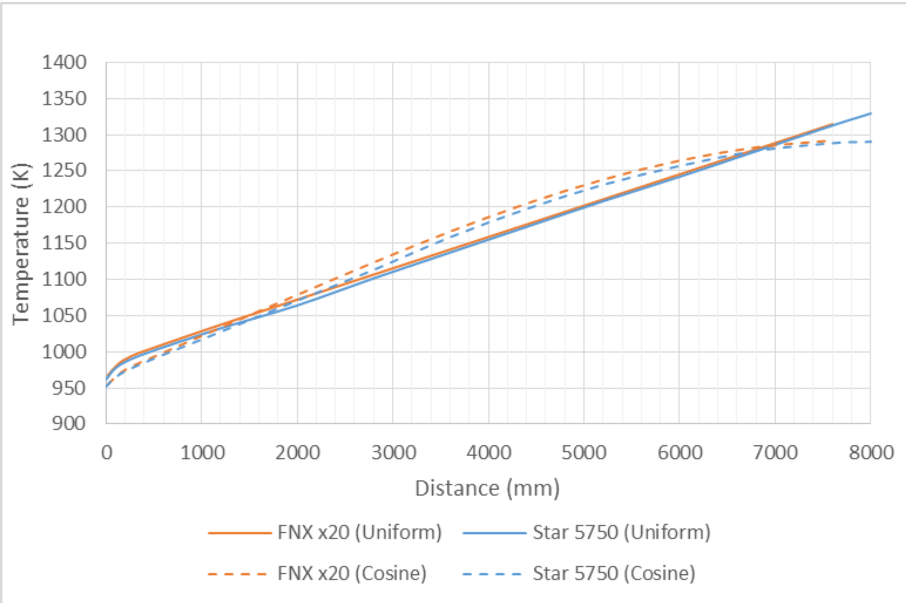


Figure 6: Fuel Compact Center Temperature (Coarse Grid)

In Fig. 6, Fig. 7, and Fig. 8 the comparison of the temperature distributions in the center of the fuel compact for the coarse, medium, and fine grids respectively are shown for the uniform and cosine power profiles. The graphs also compare the results of the temperature distribution results obtained by Flownex and STAR CCM+ with each other. As can be seen the results from Flownex and STAR CCM+ is in good agreement with each other for both the uniform and cosine power profile models.

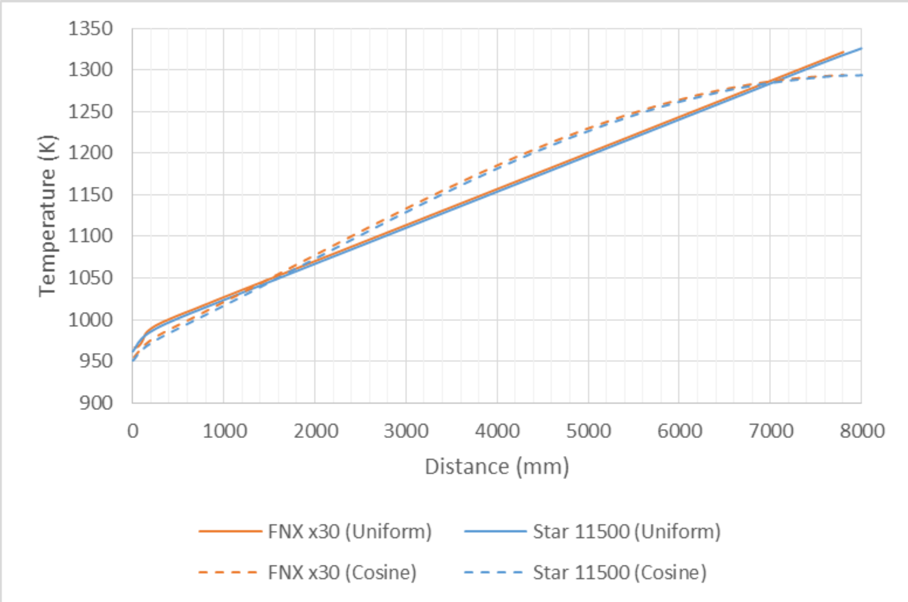


Figure 7: Fuel Compact Center Temperature (Medium Grid)

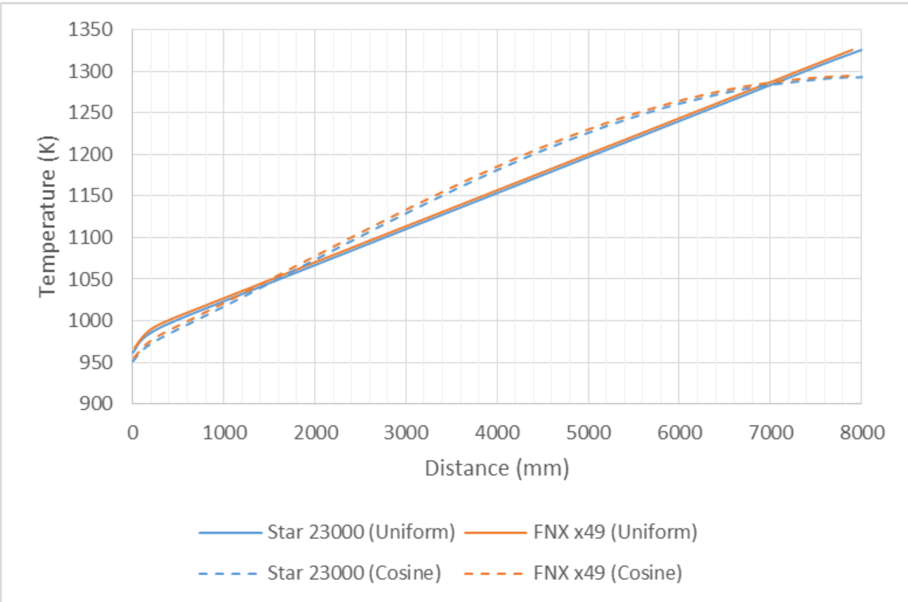


Figure 8: Fuel Compact Center Temperature (Fine Grid)

The next results consider the temperature distribution results for the fuel compact wall at the interface between the fuel compact and the moderator graphite. In Fig. 9 the results are shown for the Flownex and STAR CCM+ models which uses a coarse grid for the simulation of the two different power profiles through the SCFM. These results are in very good agreement with each other. It should also be noted that as Travis and El-Genk (2013b) no gap or resistance between the fuel compact and the moderator graphite was considered.

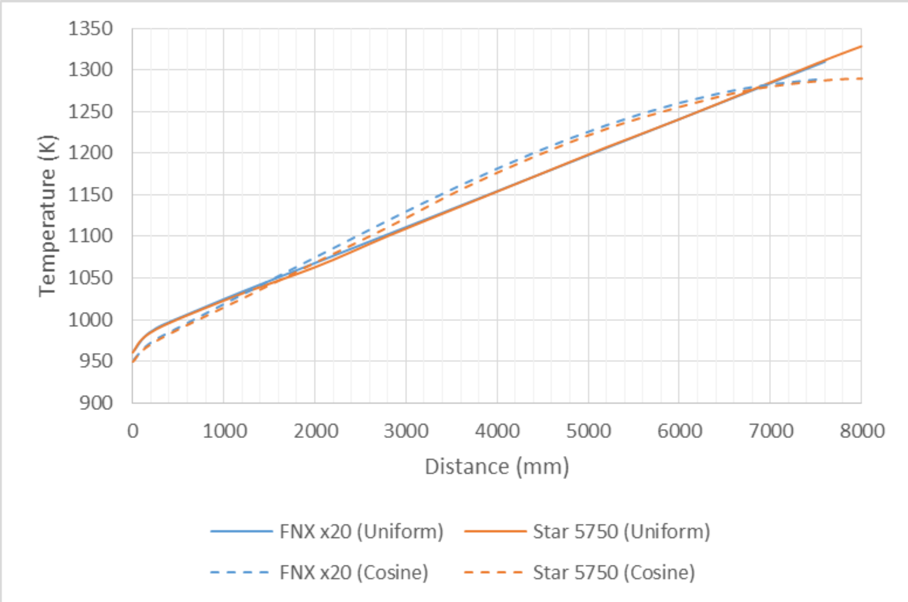


Figure 9: Fuel Compact Wall Temperature (Coarse Grid)

Fig. 10 shows the results obtained by the Flownex and STAR CCM+ medium-sized mesh model for the uniform and cosine power profiles. These results are also in very good agreement. The results obtained by Flownex and STAR CCM+ for the fine grid sized model for the uniform and cosine power profiles are shown in Fig. 11. Again, the corresponding results are in very good agreement.

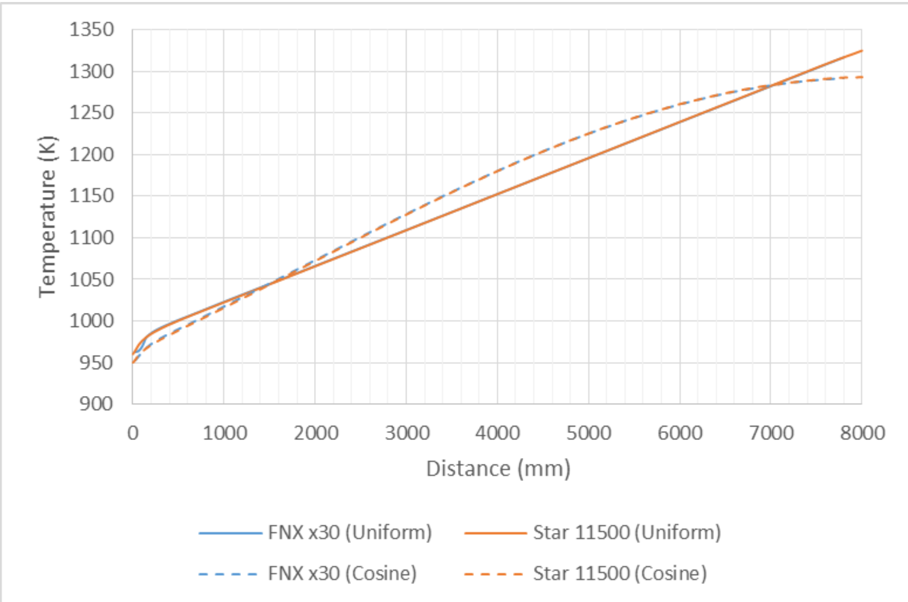


Figure 10: Fuel Compact Wall Temperature (Medium Grid)

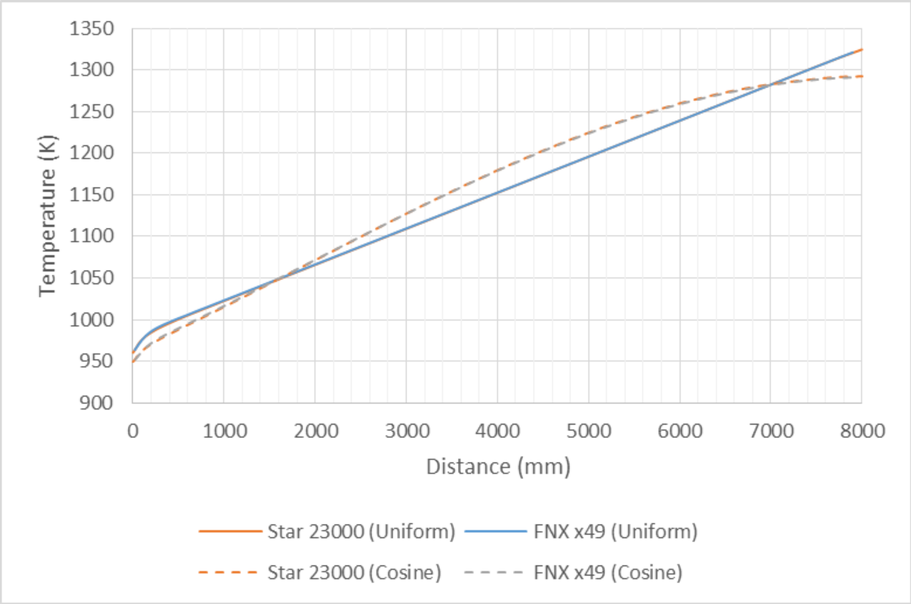


Figure 2 Fuel Compact Wall Temperature (Fine Grid)

Although not shown in the paper, it was found that the bulk temperatures of the fluid predicted by the Flownex and STAR CCM+ models were also in very good agreement.

With the results obtained by the full 1D and full 3D simulations the temperature distribution results at both the center and the wall of the fuel compact differed by less than 1%. It can therefore be concluded that the 1D Flownex models can predict the temperature distributions in the fuel compact to a very good accuracy.

6. Conclusion

In this paper, the development of a full 1D Flownex model and a full 3D STAR CCM+ model of 1/6th of a single-channel fuel module (SCFM) of a prismatic fuel block of a VHTR was discussed. The study is based on work done by Travis & El-Genk (2013b) and Nel & Du Toit (2018). A Uniform and a Cosine power profile were considered in the study. With the results obtained it is was found that the values predicted by Flownex and STAR CCM+ for the temperature distributions at the center of the fuel compact and at the wall of the fuel compact are in good agreement with each other. With the difference between the results predicted by the two codes being less than 1%, it can be concluded that the 1D Flownex models can predict the temperature distribution in the fuel compact with sufficient accuracy.

Credit authorship contribution statement

G.J. Nel: Conceptualization, Methodology, Software, Validation, Investigation, Formal analysis, Writing – Original Draft, Project administration.

O.C. Koekemoer: Conceptualization, Methodology, Software, Validation, Formal analysis, Investigation.

Prof. C.G. du Toit: Conceptualization, Supervision, Writing – review and editing. Project administration.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Nomenclature

A	Area
Ai	Aicher number
C_p	Specific heat
D	Diameter
k	Thermal conductivity
Nu	Nusselt number
Nu_{FD}	Nusselt number for fully developed flow
P	Pressure
PD	Power density
PD_{max}	Maximum power density
Pr_b	Prandtl number based on bulk fluid temperature
Ra	Rayleigh number
Re	Reynolds number
Re_b	Reynolds number based on bulk fluid temperature
R_g	Gas constant
r	Radial position
T	Temperature
T_b	Bulk fluid temperature
T_w	Wall temperature
z	Axial position
Δz	Length of increment
μ	Dynamic viscosity
ρ	Density

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