



Pin-by-pin fuel assembly coupling for North Anna PWR using Serpent and Flownex

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Abstract

This study examines the pin-by-pin fuel assembly numerical coupling of Neutronics (N) and Thermal-hydraulics (TH) in the North Anna Power Station (NAPS) Pressurized Water Reactor (PWR) core simulations to improve predictive accuracy in reactor behaviour analysis. The research focuses on developing a computational model that enhances power distribution calculations by incorporating temperature feedback effects. An external serial integration coupling strategy was applied to both the average fuel assembly and the hottest fuel assembly, utilizing Serpent for N and Flownex for TH. Results indicate that including temperature-dependent feedback yields a more accurate representation of variations within the two fuel assembly models, with standard deviations computed across all iterations of the defined fields remaining below or marginally exceeding the established convergence criterion. These results highlight the importance of coupled fuel assembly simulations in optimizing reactor safety and performance. Future research will concentrate on improving data transfer efficiency and reducing computational time for simulations.

Keywords: PWR; Flownex; Serpent; Coupling.

Acronyms

AOO	Anticipated Operational Occurrence
BDBA	Beyond Design Basis Accident
CBC	Core Critical Boron Concentration
CFD	Computational Fluid Dynamics
CPU	Central Processing Unit
DHS	Distribution Heat Source
DNB	Departure from Nucleate Boiling
DNBR	Departure from Nucleate Boiling Ratio
DBA	Design Basis Accident
DC	Doppler Coefficient
ENDF	Evaluated Nuclear Data File
ESFR	European Sodium Fast Reactor
F_Q	Total power peaking factor
FMI	Functional Mock-up Interface
GUI	Graphic User Interface
HDF5	Hierarchical Data Format 5
HPC	High-Performance Computing
k_∞	Infinite Multiplication Factor
k_{eff}	Effective Multiplication Factor
LWR	Light Water Reactor
MC/TH	Monte Carlo/Thermal-hydraulics
MDNBR	Minimum Departure from Nucleate Boiling Ratio

MOOSE Multiphysics Object Oriented Simulation Environment

MTC Moderator Temperature Coefficient

N Neutronics

N/TH Neutronics/Thermal-hydraulics

NAPS North Anna Power Station

NNR National Nuclear Regulator of South Africa

NPP Nuclear Power Plant

NWU North-West University

NWURCS North-West University Reactor Code Suite

pcm per cent mille

PVM Parallel Virtual Machine

PWR Pressurized Water Reactor

RIP Rod internal pressure

RPS Reactor Protection System

RPV Reactor Pressure Vessel

SAR Safety Analysis Report

SA Severe Accident

SCRAM Safety Control Rod Axe Man

SCWR Supercritical Water-cooled Reactors

SDM Shutdown Margin

SLFR Small Lead-based Fast Reactor

SSH Secure Shell

TH Thermal-hydraulics

UDF User-Defined Functions

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Chapter 1

Introduction

1.1 Background and rationale

The transition to sustainable energy sources contributes to addressing climate change and environmental degradation [4]. In Africa, the demand for reliable and clean energy solutions is considerable, given the increasing energy requirements and developmental goals [5].

Since 2007, South Africa has faced an increase in rolling blackouts, impacting millions and prompting discussions regarding the nation's energy future amidst an ongoing crisis [6]. The average duration of load shedding can extend up to six hours daily during Stage 6, resulting in the growing demand for sustainable energy solutions [7]. Load shedding, defined as the intentional removal of electrical supply to maintain the balance between demand and supply, has become prevalent in South Africa [8]. Eskom, which supplies electricity to 95% of the population, continues to widen the supply-demand gap annually. In addition to economic impacts, coal power plants contribute significantly to environmental degradation and climate change.

Nuclear power is an alternative energy source with the potential for stability and environmental benefits [9]. Transitioning to nuclear energy can provide a stable power supply and lower carbon emissions while facilitating technological advancement. The Koeberg nuclear power station [10], operational since 1985, contributes significantly to South Africa's energy sector, underscoring the necessity for thorough evaluation and testing of new reactor designs.

Both Koeberg and NAPS utilise PWR technology. The Koeberg reactors are based on designs adapted from Westinghouse PWR technology, similar to the technology employed at NAPS [11]. Given the inaccessibility of the Koeberg Safety Analysis Report (SAR) due to Eskom's intellectual property restrictions [12], this study will utilise insights from the NAPS PWR. Koeberg and NAPS are sister plants, sharing similar reactor designs [11]. This approach ensures the relevance and applicability of the research while addressing

intellectual property constraints. The NAPS, located in the United States, serves as a reference for this study [11].

PWRs offer several advantages that facilitate South Africa's nuclear expansion, some of which are:

- They are safe due to their inherent tendency to reduce power when the temperature increases [13].
- They can be operated with a core that contains less fissile material, reducing the risk of uncontrolled power surges [14].
- Ordinary water is used as a moderator, eliminating the need for heavy water [14].

Safety analysis in nuclear reactors, is crucial for ensuring operational safety and reducing risks to the public and the environment. The primary objective of safety analysis is to identify potential hazards and accidents that could lead to core damage or radiation release, which may affect reactor operators and surrounding communities. Risk reduction is achieved through enhancements in reactor design and the implementation of improved operational procedures. This includes systems to control reactivity changes, ensuring effective cooling systems to prevent overheating, and conducting regular maintenance and inspections. Regulatory bodies, including the National Nuclear Regulator of South Africa (NNR), require safety analyses to ensure compliance with safety standards and limits. An understanding of the interactions between N and TH is essential in evaluating safety analyses and their impact on reactor safety.

N focuses on neutron-nuclear interactions and fission chain reactions, which are essential for predicting neutron flux distribution and reactor performance. TH examines heat transfer and fluid flow within the reactor core. Understanding these processes is essential for preventing overheating and maintaining operational safety. The interaction between N and TH is significant, as neutron behaviour impacts temperature distributions, subsequently affecting reactor stability and safety margins. This research employs advanced computational methods to analyse neutron flux and heat transfer, aiming to improve reactor efficiency and safety.

This research forms part of a broader investigation into sustainable nuclear technology solutions aimed at enhancing energy innovation in Africa. The objective is to analyse the coupling of N and TH in a PWR to improve the accuracy of reactor power distribution and thermal feedback simulations. The study seeks to enhance the understanding of core behaviour under coupled conditions, thereby contributing to more reliable reactor modelling and safety analysis.

1.2 Research problem

The Fukushima nuclear disaster in 2011 emphasised the importance of understanding and mitigating Severe Accident (SA) in nuclear reactors. Furthermore, it highlighted the necessity of considering both Design Basis Accident (DBA) and Beyond Design Basis Accident (BDBA) throughout a Nuclear Power Plant (NPP)'s lifecycle.

Accurate 3D coupled N/TH calculations are necessary to ensure operational safety and flexibility. Therefore, the development of coupling methodologies is essential for thorough safety assessments.

1.3 Aim

Numerous studies have focused on the development of full-core neutron transport multiphysics systems. Conventional methods in reactor analysis often incorporate simplifications such as spatial homogenisation and energy condensation, potentially resulting in inaccuracies in the modelling of reactor behaviour [15]. Full-core multiphysics simulations mitigate these limitations by providing more detailed and realistic models. This study aims to verify and validate a N/TH model for the NAPS by modelling the full-core to ascertain the hottest and average fuel assembly powers and temperatures. This research establishes a coupling between N and TH at the pin level for both the hottest fuel assembly and average fuel assembly. The proposed methodology enhances the accuracy of simulations and contributes to a better understanding of reactor behaviour.

1.4 Objectives

The objectives of this research include the following:

1. Verify and update the existing full-core and fuel assembly N model of NAPS using Serpent to reflect the latest Westinghouse Robust Fuel Assembly 2 RFA-2 design.
2. Verify the Flownex TH model for NAPS.
3. Develop and verify a N/TH coupling methodology for NAPS.
4. Couple the hot and average fuel assemblies at a pin level.
5. Validate the model developed against the existing literature.

1.5 Dissertation structure

Chapter 2 provides a review of the literature on the coupling of TH, and N in nuclear reactor modelling. The chapter addresses the significant role of these interdependent phenomena and recent advances in multiphysics coupling analysis. Chapter 3 examines key theoretical aspects, focusing on N parameters essential for accurate reactor simulations. The chapter provides a theoretical background for parameters such as effective multiplication factor, reactivity, cross-section libraries, and computational methods, establishing a foundation for subsequent analyses. Chapter 4 outlines the methodology employed to achieve coupling, along with the verification process both during the setup phase and after coupling completion. Chapter 5 presents the findings of the coupling and conducts a critical analysis for discussion. Chapter 6 concludes the study and offers recommendations for future work to address the limitations identified.

Chapter 2

Literature Review

This chapter reviews the literature on the interdependence and implications of TH and N in nuclear core modelling. It addresses the application of computational codes in nuclear engineering and outlines advancements in multiphysics coupling analysis. Additionally, it examines various coupling strategies, numerical convergence criteria, and numerical relaxation methods, providing information on enhancing computational efficiency and accuracy in nuclear reactor models.

2.1 Introduction

N, or neutron transport theory, describes the neutron population distribution and has been a primary focus in nuclear core modelling. TH governs the temperature distribution within the nuclear fuel and influences the density and temperature fields of the moderator. These physical models are interrelated and fundamentally interdependent, affecting each other's outcomes [16].

Coupling TH and N are essential for accurately predicting coolant and fuel performance in nuclear reactor cores, particularly during accident scenarios with significant temperature variations [17]. The temperatures and densities of the moderator and fuel influence fission processes, neutron scattering (notably in the thermal and epithermal energy ranges [18]), and absorption cross-sections [19]. Increased temperatures result in decreased coolant densities, which in turn influence neutron scattering rates. Moreover, the temperature-dependent nuclear cross-sections contribute to the thermal feedback effect [20].

The Doppler effect contributes to reactor safety through negative reactivity feedback mechanisms for thermal nuclear power systems, which stabilise power output and enhance operational safety. This phenomenon occurs when changes in fuel temperature affect the neutron absorption cross-sections of the fuel material. As fuel temperature increases in response to elevated reactor power, the resonance peaks in the neutron absorption spectrum broaden. For thermal systems, with enrichment of Uranium-235 below 19.9 %, this

broadening diminishes the probability of neutron absorption by fissile nuclei, leading to a decrease in reactivity and a reduction in the potential for power excursions [21]. Consequently, the rise in reactor power leads to an increase in fuel temperature, and the Doppler effect serves to inherently counteract reactivity and power excursions by promoting neutron absorption through the broadening of resonance peaks [22]. Refer to Figure 2.1 for an illustration of Doppler broadening. However, if this feedback mechanism is insufficient and the fuel reaches the melting point, fission gases may be released from the molten UO₂. This release can cause a significant rise in internal gas pressure within the fuel pin, potentially leading to cladding rupture and fuel rod failure [23].

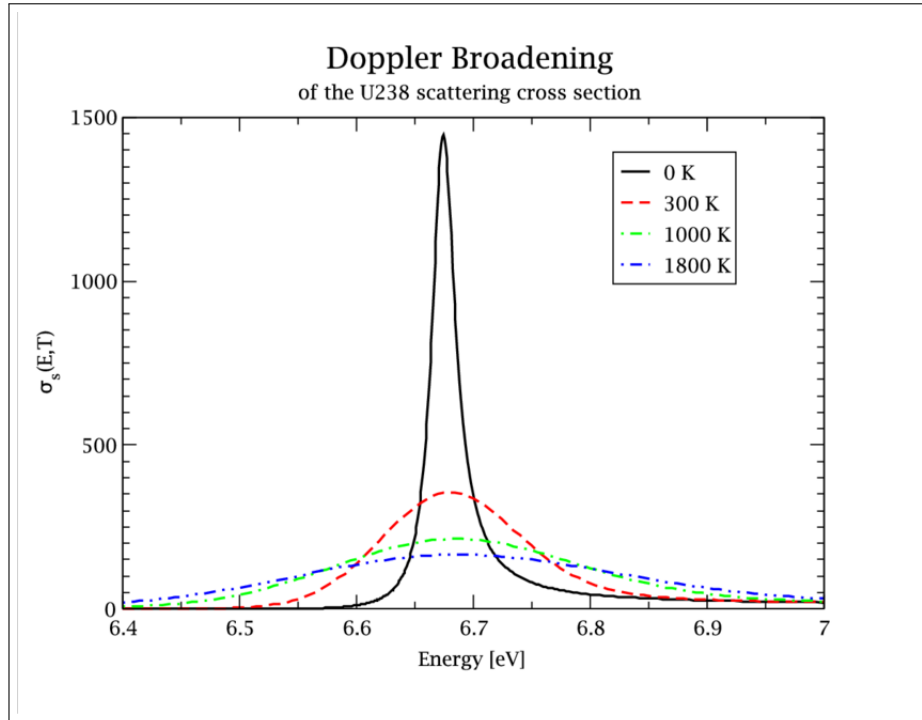


Figure 2.1: Doppler effect widening of the 6.67 eV resonance scattering cross section of ²³⁸U

[24]

The reduction in reactivity afforded by prompt, inherent negative reactivity feedback via the Doppler effect results in a decreased rate of fission reactions within the core, which mitigates undesired, rapid initial power increases. When this negative feedback operates effectively, it prevents uncontrolled increases in reactor power, ensuring that reactors remain within safety limits and minimising the risk of accidents [21]. This self-regulating mechanism allows for stable reactor output under most conditions without the need for external intervention [25]. Additionally, moderator effects, such as negative Moderator Temperature Coefficient (MTC) and negative void coefficient, may further enhance overall stability; however, these effects generally operate at a slower rate compared to the Doppler effect [22]. A large body of computational studies in reactor dynamics highlights the significance of Doppler effect feedback in maintaining safe operational conditions within a reactor.

The MTC is a measure of how changes in the moderator's temperature affect core reactivity. The influence of the moderator on reactivity is complex, involving multiple interacting factors. The density of water directly affects the reaction rate by determining the number density of scatterers. Furthermore, an interaction exists between neutron scattering and absorption in water. In borated systems, a decrease in water density correspondingly leads to a reduction in boron concentration, further influencing reactivity. Although these factors complicate the overall influence of the moderator, a negative coefficient is preferable, as it enhances the self-regulating properties of the reactor. This negative coefficient improves stability by decreasing power output when there is an unanticipated rise in temperature. Such a mechanism is crucial for controlling power surges during operational transients, thereby minimising potential accident risks. Overall, this coefficient is vital for maintaining the safety of operational nuclear reactors [26].

The Doppler temperature feedback and MTC feedback effects can be seen in this mathematical construct in Figure 2.1.

$$\begin{array}{l} T_f \uparrow \Rightarrow (n, \gamma) \uparrow \Rightarrow \phi_n^{\text{th}} \downarrow \Rightarrow (n, f) \downarrow \Rightarrow P \downarrow \\ T_m \uparrow \Rightarrow \rho_m \downarrow \Rightarrow (n' \rightarrow n) \downarrow \Rightarrow \phi_n^{\text{th}} \downarrow \Rightarrow (n, f) \downarrow \Rightarrow P \downarrow \end{array} \quad (2.1)$$

where:

- T_f = Fuel temperature
- T_m = Moderator temperature
- (n, γ) = Radiative neutron capture reaction
- ϕ_n^{th} = Thermal neutron flux
- (n, f) = Neutron-induced fission reaction
- P = Reactor power
- ρ_m = Moderator density
- $(n' \rightarrow n)$ = Neutron moderation (slowing down from fast to thermal)

In addition to nuclear effects, thermal expansion of the reactor's fuel and structural components can modify system geometry, influencing neutron transport. These structural effects, characterised by varying time constants, emphasise the importance of structural material temperatures in determining the final power distribution within the core [18]. This study, however, will not consider the thermal expansion of the reactor.

The integration of computational codes for simulating the coupled behaviours of TH and N enhances the understanding of their complex feedback.

2.2 Codes

As processing power has increased, high-fidelity nuclear reactor simulations are now feasible through multiphysics coupling analysis. The field of nuclear reactor engineering benefits greatly from advancements in computer speed and storage capacity [17, 27]. Numerical coupling between TH and N has been established, facilitating the simulation of feedback between these domains. Utilising these coupled numerical techniques allows for the simulation of interactions between TH and N within a multiphysics framework [28].

Some methods are notable, such as the development of the Multiphysics OpenFOAM solver GeN-Foam, which can solve coupled problems in parallel with various fine meshes. This development provides opportunities to describe complex processes within nuclear reactors, potentially contributing to safety and efficiency in nuclear energy applications [28].

Recently, there has been increased focus on the use of coupled TH and N codes to address nuclear reactor issues. It is important to mention that although coupling problems have been examined for an extended period, more computationally intensive methods have only recently become accessible [27].

Computer codes are utilised for various functions, including:

- Safety analysis concerning licensing and safety improvement programs for currently operating reactors
- Development of new emergency operating procedures
- Analysis of operational events
- Justification of lifetime extensions
- Improved use of nuclear fuel and increased operational flexibility
- Creation of accident management programs [29].

Hu and Uddin developed an explicit coupling technique to integrate MCNP5, a Monte Carlo neutron transport code used in reactor physics, with Fluent, utilising the User-Defined Functions (UDF). This method established the feasibility of using UDFs for field data transfer, identified as a measurable outcome of the study [30]. Cardoni demonstrated the coupling effects by analysing the 3D PWR fuel pin cell model and 3×3 model using MCNP5 and STARCCM+ coupling, yielding precise quantifications of fuel temperature, coolant temperature, density, and power distribution [31].

Yan et al. employed mesh mapping techniques to calculate the PWR 3×3 model by integrating the DeCART deterministic N code with the STAR-CCM+ TH code [32]. Using Python, Hoogenboom et al. developed a N/TH coupling method [33]. Sjenitzer et al. [34] presented a method for transient coupling with the Monte Carlo code. Ward et

al. simulated the safety performance of the I2S-Light Water Reactor (LWR) plant under accident conditions using the coupled system code RELAP5 and the 3D spatial kinetics code PARCS [35].

With the advancement of computational codes, the integration of these tools into coupling methodologies is necessary. Such methodologies are critical for simulating the interactions in nuclear reactors and form the basis of the coupling methods discussed in Section 2.3.

2.3 Coupling methods

Reviewing past studies, there has been a trend of combining deterministic N codes with their TH counterparts. Examples include coupling the WIMSD5 and CITATION codes with COBRA-EN [29], PARCS with RELAP5 [36], and RAST-K with CTF [19]. Research has also focused on merging Monte Carlo N codes with TH code, such as MCNPX with COBRA-IV-I [18] and MCNP5 with SUBCHANFLOW [37]. These investigations demonstrate the multidisciplinary nature of nuclear core modelling and the challenges in achieving comprehensive simulations that accurately represent the interactions between different physical phenomena.

2.3.1 Coupling interface

Coupling interfaces facilitate communication and data exchange between various N codes or between N and other physical phenomena, such as TH. These interfaces ensure the effective integration of codes while preserving stability and accuracy.

2.3.2 Types of coupling

The primary methods for coupling TH codes with N codes are external, internal, and hybrid coupling.

External Coupling: This method involves executing codes separately and utilising external scripts or platforms to manage their interactions. It is straightforward to implement as it necessitates minimal modifications to the existing codes, although it may lack flexibility. A user interface module enables the codes to operate independently during this process. For example, the UDF interface was developed to facilitate data exchange between Fluent and an unspecified Monte Carlo simulation code, enhancing management. The UDF module maps Monte Carlo code cells with Fluent meshes. The Monte Carlo code provides a heat source term to the Fluent meshes, while the Fluent results update the temperature and density for the Monte Carlo code, leading to the modification of cross-sections in the input file with each iteration [17]. Although external coupling provides simplicity and modularity, its dependence on disk-based data transfer reduces efficiency for reactor sys-

tems that require rapid feedback and strong integration between physics domains, leading to slower convergence [38].

Internal Coupling: This approach integrates the codes into a unified system, necessitating modifications but providing enhanced flexibility. In this configuration, data exchange occurs within the integrated code, facilitating improved parallel computing and accuracy, despite requiring considerable code adjustments. Both source codes must be available, and users must have advanced coding capabilities [39].

Hybrid Coupling: As explained by Shang, this method addresses the challenges of Monte Carlo/Thermal-hydraulics (MC/TH) coupling through the integration of external and internal strategies. It seeks to optimise usability and functionality by mitigating the limitations of each individual approach [40]. By merging aspects of both, the hybrid approach offers an efficient means to simulate complex reactor phenomena, streamlining the process while preserving adaptability [41].

2.3.3 Execution strategies

Serial Integration Coupling: This method modifies the source code to integrate N and TH systems. It maintains one code static while another, such as the neutron kinetic code, executes. The running code generates power distribution data, which is used by the static TH code to calculate various parameters [42]. The data is then cycled back to update the neutron kinetic code, perpetuating the process.

Parallel Coupling: This technique allows codes to operate independently while exchanging data during calculations within a Parallel Virtual Machine (PVM) environment. It facilitates simultaneous computations of N and TH, improving data exchange efficiency and computational parallelism [42]. This coupling reduces overall simulation time and improves convergence rates. A study by Gaston demonstrates the Multiphysics Object Oriented Simulation Environment (MOOSE) framework that utilises parallel computational hardware to connect various domain-specific applications, highlighting an increase in simulation speed as observed in the KAIST-3A benchmark core and the Westinghouse AP-1000 configuration [43].

A study conducted by Khan [44] identified challenges associated with the implementation of parallel coupling as an execution strategy. One such challenge is the inter-process communication overhead, which limits the effectiveness of the method based on the number of Central Processing Unit (CPU)s utilised. The introduction of parallelisation increases program complexity, complicating understanding, debugging, and maintenance. Consequently, this necessitates additional time investment in program design and debugging, which may offset the advantages of parallelisation. As a result, this can lead to inaccuracies in outcomes and an increase in computational time required for simulations.

2.3.4 Case study: Coupling of DRAGON/DONJON and COBRA codes for SMART reactor

An example of integrated coupling is the research conducted by Akbari et al. [45], which focuses on the SMART reactor, an integrated PWR reactor. Using an integrated nuclear code coupling method, this study analyses various thermo-neutronic characteristics.

N Core Calculations: N cell computations employ the DRAGON code, which uses homogenisation techniques to reduce computational volume and generate multigroup cross-section tables. Subsequently, the DONJON code utilises these homogenised parameters for core-level N analyses.

TH Calculations: COBRA is a sub-channel code used to simulate coolant flow and heat transfer in fuel rod bundles. It generates data related to TH properties, including coolant pressure and temperature.

Results and Discussion: The coupling of DRAGON/DONJON and COBRA codes was verified against independent calculations, demonstrating improvements in accuracy. By coupling N and TH aspects, a more precise understanding of the power distribution and thermal behaviour of the reactor core was obtained.

Integrated Coupling Process:

1. Collect input data for DRAGON, DONJON, and COBRA codes.
2. Make initial guesses for temperature and density distributions.
3. Execute DRAGON, extract outputs, and input into DONJON.
4. Perform N calculations, and extract power coefficients.
5. Execute COBRA for TH calculations.
6. Iteratively adjust inputs and assess convergence.

Conclusion: This case study demonstrates that reliance on stand-alone code modelling is less efficient compared to a coupled approach for N and TH data exchange. The coupled approach provides more precise predictions of reactor behaviour, which is essential for understanding reactor operations and preparing for non-ideal scenarios encountered during routine operations. Feedback mechanisms between N and TH are significant, as N calculations utilise temperature and density distributions obtained from TH calculations. Conversely, TH parameters are influenced by power distributions established by N. To improve accuracy in research, it is imperative to facilitate data exchange between codes during simulations, rather than relying exclusively on either N or TH.

Coupling N and TH during burnup calculations improves the representation of power and thermal distribution, leading to enhanced predictions of cycle length. In the case of the

SMART reactor, stand-alone calculations indicate a cycle length of 863 days. However, the coupling procedure yields a cycle length of 891 days, which aligns closely with the designer's specified cycle length of 900 days as reported in SMART documentation [46]. The use of a SAR in this study further supports these findings, indicating that the integration of N and TH enhances accuracy in relation to the reactor's design parameters.

The assessment of coupled versus non-coupled parameters demonstrates that average outcomes from both methodologies are satisfactory, see Figure C.1. However, the lack of a coupling procedure for specific parameters, such as Minimum Departure from Nucleate Boiling Ratio (MDNBR), leads to significant deviations when compared to results obtained from the coupled approach. The relative maximum difference observed for the MDNBR parameter at the bottom of the core between coupled and non-coupled modes is 15.9 %, see Figure C.2. For the Effective Multiplication Factor (k_{eff}) value, a difference of 513 pcm is noted between the coupled N (1.000593) and non-coupled N (1.005724) values, as depicted in Figure C.3. These findings illustrate that the coupling of N with TH can significantly influence reactor behaviour. Thermal feedback mechanisms, including Doppler broadening and coolant density changes, influence reactor criticality and highlight the necessity of coupling N with TH for accuracy in reactor simulations. In other words, modelling TH feedback impacts the computational fidelity and validity of the modelling of reactor behaviour.

In conclusion, coupling provides a more realistic and valid modelling of the reactor core, which enhances the safety of nuclear reactors - there will be a better correspondence between modelling predictions and actual reality. This research aims to achieve similar objectives 1.3.

2.4 Coupling levels across geometric scales

In multiphysics reactor simulations, particularly those involving the coupling between N and TH, the level of coupling and geometric scale significantly influence both model fidelity and computational cost. Coupling levels describe the resolution and depth of data exchange between solvers, while geometric scale refers to the physical extent of the domain being modelled, such as the full core, a single fuel assembly, or an individual fuel pin.

2.4.1 Definition of coupling levels

Coupling levels can be broadly categorised as follows:

- **Core-Level Coupling:** A single TH channel represents the entire reactor core. N and TH solvers exchange aggregate parameters such as total core power and average coolant temperature or density.

- **Fuel Assembly-Level Coupling:** Each fuel assembly is modelled with an independent TH channel. Power distributions and coolant flow characteristics are resolved at the assembly level, improving spatial accuracy relative to core-level models.
- **Pin-Level Coupling:** Each individual fuel pin is modelled with a separate TH channel. Power and thermal feedback are resolved on a pin-wise basis, allowing for detailed simulation of intra-assembly power distribution and thermal gradients. This level captures detailed phenomena such as cladding behaviour and localised hot spots.
- **Subpin-Level Coupling:** Also known as subchannel coupling. This is the most detailed coupling, where intra-pin regions (e.g., axial slices, radial segments, or angular wedges) are individually modelled. This level captures the overall coolant flow distribution and thermal conditions in the coolant channels, enabling the analysis of inter-channel flow mixing, pressure drops, and localized temperature variations across the fuel assembly.

2.4.2 Geometric model sizes

Geometric scales in reactor modelling can be defined as:

- **Full Core:** Encompasses the entire reactor core, typically consisting of numerous assemblies.
- **Fuel Assembly:** Represents a single assembly, such as a 17×17 fuel rod lattice.
- **Fuel Pin:** Models a single fuel rod, which may include hundreds of such pins per assembly.

2.4.3 Coupling level implementation by geometric scale

Full Core Simulations

- **Core-Level Coupling:** N provides total core power. TH models the core as a single channel, returning bulk-averaged coolant properties. This method is computationally efficient but lacks local resolution.

Fang et al. present a full-core N/TH coupling study for a Small Lead-based Fast Reactor (SLFR). Discrete ordinate nodal method for N is used, and a parallel channel model for TH, where each hexagonal fuel assembly is treated as one channel. This corresponds to core-level coupling with aggregated data exchange representing the full core in TH. The coupling is done via power distribution and temperature-dependent cross sections with a loose internal coupling strategy, iterated to convergence. They found that maximum temperatures of fuel, cladding, and coolant stayed within design limits. The maximum fuel temperature and cladding temperature values were

not explicitly listed but were confirmed safe under the modelled conditions. TH feedback induced a negative reactivity feedback (~ -200 pcm) with minor impact on power distribution ($<1\%$). The coolant temperature distribution was computed with axial convection and showed moderate gradients consistent with operating limits. The iterative coupling between N and TH converged rapidly, demonstrating stable coupled solutions [47].

- **Assembly-Level Coupling:** TH supplies per-assembly power distributions. TH models each assembly as a distinct channel, enabling improved resolution of radial and axial effects.

Fang et al. also describe assembly-level coupling where N provides power per assembly, and TH solves coolant temperature and flow separately for each assembly channel, giving better axial and radial resolution than core-level. Using a similar approach, Wang et al. also modelled fuel assembly-level coupling, which gives better axial and radial resolution. This improved temperature detail within assemblies, again showing maximum temperatures within operational specifications, but detailed numeric maximum temperatures were not specified [47].

- **Pin-level Coupling:** N generates individual pin powers. TH computes flow and heat transfer per pin. This increases accuracy but significantly raises computational demands.

A review study on N/TH coupling methods discusses high-fidelity pin-by-pin coupling where each fuel pin has its dedicated TH channel. This allows detailed, accurate heat transfer and flow modelling but is computationally expensive. Such studies typically involve coupled N, TH, and fuel performance codes for safety analyses. Reviews and multi-physics studies emphasise that pin-by-pin coupling enables resolving local hot spots and temperature gradients in each fuel rod. Temperatures here are found with high spatial resolution and typically show increased maximum fuel temperatures compared to coarser models, important for safety margins [48].

- **Subpin-Level Coupling:** N provides detailed intra-pin power distributions. TH resolves pellet-scale variations, cladding behaviour, and coolant interactions. Typically applied in high-fidelity simulations or safety validation studies.

High-fidelity multiphysics coupling at the subpin level is used for intra-pin spatial variations, including pellet and cladding layers. This is described in an OECD NEA report, outlining ultra-detailed coupling with multi-physics solvers, used for benchmark and accident scenario studies. This ultra-detailed modelling captures radial and angular temperature gradients within a rod, reporting peak temperatures often near safety limits. Precise temperature values depend heavily on scenario; however, peak clad temperatures typically remain below ~ 1200 K in normal operation, with fuel centerline temperatures being higher. These models support accident and transient analyses where local thermal phenomena dominate [49].

- **Assembly-Level Coupling:** Treats the entire assembly as a homogenised region. N provides integrated power, while TH returns average coolant properties. Used for simplified or preliminary analyses.

Ye et al. present a N/TH coupling study on a plate-type fuel assembly using Fluent and Monte Carlo codes. The coupling at the assembly level treats all rods lumped together, modelling reactor core physics and TH at the assembly scale. This approach allows studying blockage accidents and overall assembly behaviour. This study found that in coupled simulation the assembly fuel temperatures rose approximately 30 ° C when coolant blockage occurred, indicating that the coupled model can accurately capture temperature homeostasis and response to TH effects [17].

- **Pin-level Coupling:** Power and thermal feedback are resolved per rod. Enhances fidelity for local performance assessments or benchmarking studies.

Studies implementing pin-by-pin coupling within a single assembly model individual rods with N providing power per rod and TH giving rod-specific coolant conditions. Such analyses are commonly featured in high-fidelity codes used for detailed assembly simulations and hot spot identification, as discussed in high-level reviews. Studies highlighted in reviews indicate pin-by-pin coupling within an assembly yields more precise temperature distributions, resolving hot rods and local peak fuel temperatures. Typical values for normal operation are consistent with full core pin-level results (~700–1200 K fuel temps) [48].

- **Subpin-Level Coupling:** Captures detailed spatial behaviour within each pin. Enables analysis of fine-scale effects such as fuel cracking, localised overheating, or Departure from Nucleate Boiling (DNB).

Single-pin simulations

- **Pin-level Coupling:** The entire pin is modelled as a 1D or 3D TH domain. N provides total pin power. Commonly used for fuel performance or burnup analyses.

Maximum fuel temperatures can vary depending on power, but typical operational ranges are again a few hundred degrees Celsius below melting points [48].

- **Subpin-Level Coupling:** N delivers detailed intra-pin power profiles. TH resolves radial conduction, cladding-to-coolant heat transfer, and fuel-cladding gap behaviour. Essential for transient analyses and safety margin evaluations.

2.4.4 Computational considerations and use cases

As the coupling level increases from core to subpin, the computational requirements increase significantly. The selection of an appropriate coupling level is driven by the objectives of the analysis:

- Core-Level: Suitable for design scoping or control studies.
- Assembly-Level: Used for operational support or steady-state analysis.
- Pin-by-Pin: Required for core optimisation, power peaking studies, or fuel management.
- Subpin-Level: Necessary for safety analysis, accident modelling, and validation against experimental data.

Subpin-level coupling is frequently integrated with multi-physics frameworks, combining N, TH, and fuel performance solvers. This enables predictive capabilities for complex phenomena under normal and off-normal conditions.

2.4.5 Comparison of reactor coupling methods

To understand reactor coupling methods and their applications, see Table 2.1. This table details the N and TH codes used, the reactors to which they are applied, the coupling methods employed, and the level of coupling achieved. This comparison enables an understanding of how different approaches are utilised across various reactor types and scenarios, highlighting the adaptability of coupling strategies in nuclear engineering.

Coupling level & size	Neutronics code(s)	Thermal-Hydraulics code(s)	Coupling Type (Internal/External)	Type of reactor	Reference
Full core, Core-level coupling	Discrete ordinate nodal method (not explicitly named code)	Parallel channel model (custom/in-house)	Internal coupling (loose) (in-memory exchanges iterative)	SLFR	[47]
Full core, Assembly-level coupling	Discrete ordinate nodal method (not explicitly named code)	Parallel channel model per assembly (custom/in-house)	Internal coupling (loose)	SLFR	[47]
Full core, Pin-by-pin coupling	Not explicitly named	Not explicitly named	Internal coupling (usually tight, tightly integrated)	Various (often fast reactors)	[48]
Full core, Subpin-level coupling	Not explicitly named	RELAP5, TRACE, fuel performance codes (e.g., FRAPCON)	Internal coupling (tight multiphysics integration)	LWRs	[49]
Fuel assembly, Assembly-level coupling	Monte Carlo method (general, no explicit code name)	Fluent Computational Fluid Dynamics (CFD)	External coupling (file/API based exchange between separate codes)	Plate type reactor fuel assembly (research model)	[17]
Fuel assembly, Pin-by-pin coupling	Not explicitly named	Not explicitly named	Internal coupling (usually tight)	Various assembly simulations	[48]
Fuel assembly, Subpin-level coupling	Not explicitly named	RELAP5, TRACE, fuel performance codes	Internal coupling (tight multiphysics integration)	LWR fuel assembly	[49]
Single pin, Pin-by-pin coupling	Not explicitly named	Not explicitly named	Internal coupling (usually tight)	Single fuel pin	[48]
Single pin, Subpin-level coupling	Not explicitly named	Fuel performance codes such as FRAPCON, TRANSURANUS	Internal coupling (tight multiphysics)	Single fuel pin	[49]

Table 2.1: Reactor coupling methods comparison table

Based on Table 2.1, a comparison of various studies has been conducted regarding the coupling between N and TH codes. This analysis details the codes utilised, reactor types examined, coupling methods implemented, and the precision achieved in coupling. The findings reveal that most pin-level multiphysics approaches employ internal coupling, where N and TH solvers exchange data directly within an integrated environment. However, external coupling remains a viable alternative when the solvers involved are independent, specialised tools.

A study focused on coupling Serpent and Flownex at a pin-by-pin level within a fuel assembly can leverage established methodologies from previous research. For instance, [50] successfully implemented full-core pin-by-pin coupling utilising OpenFOAM and CorTAF. Similarly, Kim [39] employed the iMC code in conjunction with a three-dimensional finite element method to achieve internal pin-by-pin coupling. Additionally, García-Herranz [51] attained pin-by-pin resolution through external coupling with COBAYA and CTF. This study builds upon previous research, such as that by Du Toit [52], which coupled Serpent and Flownex on an average pin model. However, the existing literature lacks documented external coupling between Serpent and Flownex on a fuel assembly pin-by-pin basis, indicating that this research could offer novel insights.

External coupling of Flownex and Serpent at the pin-by-pin level will enable the utilisation of each code's core strengths without requiring extensive code modification or integration into a common framework. Serpent offers high-fidelity Monte Carlo N with flexible geometry modelling and accurate pin-wise power distributions. Flownex provides advanced TH network modelling with robust transient and steady-state capabilities. Through external coupling, pin power distributions from Serpent can be transferred to Flownex for detailed coolant and fuel temperature calculations, while temperature and density feedback from Flownex can be reintroduced into Serpent for updated neutronic calculations.

2.5 Convergence criterion

Convergence occurs when the relative temperature difference between the current and previous iterations is below a predetermined threshold [18]. If the temperature difference meets this threshold, other parameters such as power distribution may be deemed acceptable. Otherwise, calculations continue with updated temperature values until the difference between recent iterations falls to an acceptable level [29].

2.5.1 Convergence of thermal-hydraulics codes

Accurate and stable simulations when coupling N and TH require TH codes to achieve convergence. TH calculations provide temperature, density, and flow distributions, which have a direct influence on neutron cross-sections and power generation in neutron codes. Non-converged TH results may lead the N solver to process inconsistent data, resulting

in oscillations or divergence in the coupled simulation. The implicit coupling method, commonly utilised for multiphysics problems, involves iterative data exchanges between codes to achieve convergence at each time step. Starting with a converged TH solution reduces the number of iterations necessary for global convergence [53].

2.5.2 Source convergence in Monte Carlo simulations

In Monte Carlo simulations, source point convergence is essential for stabilising the fission source distribution across iterations. The convergence of the source point directly influences k_{eff} and significantly impacts the understanding of system behaviour under various conditions, which is critical for safety assessments.

Shannon entropy was introduced in MCNP5 to function as a metric for assessing the convergence of the fission source. This implementation was further improved in the MCNP6 codes [54]. The Serpent Monte Carlo code also produces a Matlab-readable results file "res.m" containing simulation outputs, including entropy-related data [55]. It signals that the counting process is complete when the fission source attains a state of convergence. This entropy measure quantifies the convergence of the fission source distribution, reaching a steady-state value as the distribution approaches stationarity [56]. The initial source distribution is determined by MCNP using TH feedback, which applies a homogeneous radial power profile together with an axial power profile to facilitate convergence. [37].

A review of existing convergence criteria identifies several methods that can enhance source convergence in Monte Carlo simulations. These methods include eigenvalue convergence, flux-based convergence, assessment of local fuel temperature, evaluation of local power distribution, and Monte Carlo uncertainty analysis. Each method presents specific advantages and challenges, necessitating meticulous evaluation to determine their effectiveness in achieving convergence [57].

2.5.3 Neutronics/Thermal-hydraulics coupling convergence

N/TH coupling convergence denotes the stabilisation of solutions during the integration of the N system, which involves neutron behaviour and reactions, and the TH system, addressing fluid dynamics and heat transfer. This integration is necessary for accurate simulations of nuclear reactors. Convergence is generally achieved using iterative methods, such as Picard iteration, where each system is solved independently before data is exchanged until both solutions stabilise within defined tolerances.

Zahur utilised the Picard convergence method during each burnup phase to attain convergence for multiple parameters. These parameters included moderator density, fuel temperatures, cladding temperatures, boundary conditions for both moderator and coolant, linear power, and film heat transfer coefficients [19]. The non-linear characteristics of the coupled physics necessitate multiple iterations to obtain a converged solution [37]. The Pi-

card iteration method effectively addresses non-linearities while maintaining the accuracy of high-order time schemes. To mitigate computational costs, convergence acceleration is essential, as iteration at each time step can be resource-intensive [16].

Issues have been identified with this method. While it is suitable for implementation in coupled reactor simulations, challenges such as potential instability without appropriate relaxation factors and slower linear convergence rates, compared to advanced techniques that dynamically integrate feedback, have been observed [58], [59]. Additionally, computational errors can occur due to iterative data exchange among multiple coupled codes that utilise various techniques. Minimising these errors requires reducing the acceptable error threshold, which may extend the time required to achieve convergence [29].

2.6 Relaxation

In numerical methods, a relaxation parameter (often denoted by ω) is a value, typically between 0 and 2, used to adjust the step size in iterative methods to accelerate convergence. By multiplying the update step by this parameter, the method can either “over-relax” ($\omega > 1$) or “under-relax” ($\omega < 1$) the solution, impacting stability and convergence. This method reduces fluctuations between iterations, lowering the risk of divergence caused by strong non-linear changes. In N/TH coupling, experience shows that it is vital to select $\omega \lesssim 0.5$ to ensure numerical stability and convergence.

Relaxation modifies the iterative function to satisfy convergence criteria, making fixed-point iteration an effective method for achieving convergence [60]. This technique promotes gradual changes in power and temperature throughout the iterations, thereby enhancing the stability of convergence.

2.6.1 Fixed relaxation

Fixed relaxation employs a constant under-relaxation factor throughout the iterations of simulations. This factor influences the transfer of data from one iteration to the next as the solvers exchange information. The primary aim of fixed relaxation is to reduce the potential for oscillations or divergence that may occur if information is utilised without applying the factor. By limiting changes between iterations, this method improves stability and facilitates convergence towards a solution.

A study [61] utilised coupled Serpent and OpenFoam with Picard iterations and a power relaxation factor. Various values for the relaxation factor were evaluated: $\alpha = 1$ (without relaxation), $\alpha = 0.25$, and $\alpha = 0.1$, in order to determine the most effective option. The relaxation factor $\alpha = 0.1$ demonstrated optimal convergence after two iterations, while $\alpha = 1$ achieved a relative power of 1 % after 24 iterations. The power flux for TH simulations q_n is derived from the power flux predicted by the Monte Carlo simulation q_n^* and the

power flux from the prior iteration step q_{n-1} . The relaxed power flux was calculated as:

$$q_n = \alpha q_n^* + (1 - \alpha)q_{n-1}, \quad (2.2)$$

where α denotes the relaxation factor.

This study [61] indicates that a lower relaxation factor can improve the convergence rate of predicted linear power. However, simulations that utilise a relaxation factor that is excessively low may result in unconverged velocity and temperature fields, which is associated with the damped power difference and the corresponding TH feedback. In contrast, excessively high values of the relaxation factor may induce oscillations, indicating instability, as shown in Figure C.5. These findings highlight the necessity of selecting an appropriate relaxation factor, which may require several trials.

The advantages of this relaxation method include its simplicity, maintenance of stability, and constancy of factors throughout simulations. A notable disadvantage is its potential inability to consistently achieve optimal convergence rates compared to adaptive methods, which will be further explored in the subsequent subsections.

2.6.2 Varying relaxation factor using stochastic approximation

This method adjusts parameters, including relaxation factors, during iterative processes. The approach is useful when optimal parameter values are not predetermined or when processing noisy data, which includes errors or unwanted variability. Stochastic approximation is utilised for iteratively updating estimates based on these noisy observations. In relation to varying relaxation, the method entails modifying the relaxation factor, such as the under-relaxation factor, at each iteration in response to prior feedback.

A study by Korinek [61] indicates that fixed relaxation factors can stabilise coupled simulations, although they may result in slow convergence. It is proposed that a varying relaxation factor, computed using Equation 2.3 and refined through stochastic approximation, could enhance performance regarding stability and convergence speed. The relaxation factor is calculated as:

$$\alpha_n = \frac{s_n}{\sum_{i=1}^n s_i}, \quad (2.3)$$

where s_n denotes the quantity of simulated particles and α_n indicates the relaxation factor at iteration n .

The advantages of this relaxation method include the capability to make real-time adjustments based on previous iterations, the ability to mitigate the impact of noisy data through average error reduction across iterations, and the potential for faster convergence in com-

parison to fixed methods due to dynamic parameter adaptation. However, a limitation of this approach is that the implementation of stochastic approximation requires a comprehensive understanding and knowledge of both the relevant physics and the associated statistical methods involved.

2.6.3 Self-adaptive relaxation

Smaller relaxation factors can enhance convergence rates while potentially increasing computation times. Traditionally, the selection of these factors is performed manually based on experience, which can be inefficient, especially for reactors with complex N/TH interactions such as Supercritical Water-cooled Reactors (SCWR) [60].

To address these challenges, Liu presents a self-adaptive relaxation factor based on the contraction principle. This method adjusts the relaxation factor dynamically, utilising feedback from previous iterations, including residual values and convergence rates. The convergence analysis presented in the study demonstrates that the self-adaptive relaxation method improves computational efficiency compared to conventional methods. This approach serves as a practical alternative to manual selection processes. For a comprehensive overview of the methodology, refer to Figure C.4 [60].

2.6.4 Conclusion

Based on the general consensus of other researchers, as well as personal experience, this study employs fixed relaxation for power and temperature as the chosen method due to its simplicity. The method involves applying a constant fraction of calculated changes at each iteration, which facilitates coding and debugging. In contrast to adaptive methods that necessitate extra calculations to adjust the relaxation factor based on current conditions, the fixed approach minimises this additional computational load. This method is efficient in decreasing computational time.

2.7 Conclusion

This literature review outlines findings related to the mutual influence of N and TH on reactor outcomes, focusing on the interactions of these phenomena within the reactor. N and TH are critical for predicting reactor coolant behaviour and overall performance. The coupling of N and TH enhances the accuracy of reactor behaviour predictions, resulting in improved estimates of the design parameters as listed in the SAR and safety analysis compared to independent analyses. Most coupled simulations in the literature are conducted externally, likely due to the higher computational costs associated with internal coupling. However, external coupling often requires numerous iterations to achieve convergence, which can extend computational times. The reviewed studies underscore the roles

of Shannon entropy and relaxation methods in maintaining reactor stability and convergence, as well as the importance of negative reactivity feedback from the Doppler effect in improving reactor safety.

This dissertation examines the coupling of N and TH in a PWR to improve the accuracy of reactor behaviour simulations, thereby enhancing the understanding of core performance and safety analysis. Existing literature lacks a comprehensive study that couples Serpent and Flownex at the pin-by-pin level, which may provide important insights into reactor dynamics. Establishing pin-by-pin coupling requires alignment of the model geometry with the actual reactor geometry, as specified in SAR. The objective of the research is to validate the coupled model for both the hottest and average assemblies at the pin-by-pin level, employing an external serial integration coupling strategy with fixed relaxation of temperature and power. This approach involves sequential processing of one model, using its outputs as inputs for the subsequent model.

The subsequent chapter will examine the theoretical framework necessary for a comprehensive understanding of N, TH and coupling along with the relevant equations.

Chapter 3

Theory

This chapter presents the theoretical background of N parameters that contribute to the foundational theories relevant to coupling.

3.1 Neutronic parameters

N parameters are critical factors in the coupling of codes in nuclear engineering because they influence simulation accuracy, efficiency, reliability, safety, and regulatory compliance. Effective representation and management of these parameters are necessary for obtaining accurate and reliable coupled simulations of nuclear reactors.

3.1.1 Effective multiplication factor

The multiplication factor represents the ratio of neutrons produced/absorbed/lost in one generation to those produced/absorbed/lost in the previous generation. k_{eff} serves as a critical indicator of nuclear reactor criticality [62].

Mathematically, the equation for the k_{eff} is represented as Equation 3.1.

$$k_{\text{eff}} = \frac{\text{Neutron production rate}}{\text{Neutron absorption rate}} \quad (3.1)$$

Here are the typical values and their implications:

- $k_{\text{eff}} = 1$: The reactor is critical, meaning the number of neutrons produced is equal to the number of neutrons lost, leading to a stable reaction.
- $k_{\text{eff}} > 1$: The reactor is supercritical, indicating that the number of neutrons produced exceeds the number of neutrons lost. This situation can lead to an increasing neutron population and a potential power excursion if not controlled.

- $k_{\text{eff}} < 1$: The reactor is subcritical, meaning that the number of neutrons produced is insufficient to sustain a chain reaction, leading to a decrease in neutron population.

Control of k_{eff} is essential in nuclear reactors to ensure safe and stable operation. Reactor operators adjust control rods, which absorb neutrons, to maintain k_{eff} at or near 1 for sustained and controlled power generation.

3.1.2 Infinite multiplication factor vs. effective multiplication factor

Infinite Multiplication Factor (k_{∞}) refers to the N parameter associated with an individual fuel assembly, assuming no neutron leakage. This situation is modelled using reflective boundary conditions, which simulate an infinite lattice and prevent lateral neutron escape. Within this framework, the fuel assembly operates as if it is part of an infinite array, thus facilitating the calculation of k_{∞} .

In contrast, k_{eff} represents the effective neutron multiplication factor for the entire reactor core, accounting for both neutron production and losses due to leakage and other systemic effects. While both k_{∞} and k_{eff} are N parameters, they fulfill different roles in reactor physics: k_{∞} represents an idealised, leakage-free state, whereas k_{eff} captures the actual operational conditions of a finite nuclear system.

For the study and measurement of neutron behaviour within a reactor core, the Four-factor Formula serves as a fundamental concept in nuclear reactor physics [63]. The process of neutron chain reaction is governed by four key components, which include:

1. **Reproduction factor (η):** It is defined as the ratio of the number of thermal neutrons absorbed by the fuel to the number of fast neutrons produced by thermal fission [64].
2. **Thermal utilisation factor (f):** The ratio of the total number of thermal neutrons absorbed within the fuel (including all nuclides) to the total number of thermal neutrons absorbed within all materials comprising up the reactor core [65].
3. **Resonance escape probability (p):** This quantifies the likelihood of a neutron avoiding absorption within the resonance energy range, typically between 2 MeV and 10 eV, as it transitions to thermal energies. In LWRs, neutrons begin at elevated energies, approximately 2 MeV, and require moderation to energies below around 10 eV, where the fission cross section $\sigma_{(n,f)}(E)$ becomes significant. The energy interval includes multiple capture resonances, leading to non-fission neutron absorption via (n, γ) reactions. A heterogeneous fuel-moderator configuration improves resonance escape probability by enabling fast neutrons to exit the fuel prior to entering the resonance energy region. These neutrons then scatter within the moderator and frequently re-enter the fuel at lower, sub-resonance energies. Such spatial separation

between the fuel and moderator minimises neutron losses, thereby improving the resonance escape probability [66].

4. **Fast fission factor (ϵ):** It is defined as the ratio of the total number of neutrons generated from all fissions, including those induced by fast neutrons, to the number of neutrons produced exclusively by thermal fissions. This factor quantifies the contribution of fast fissions to the overall neutron economy, facilitating the total number of neutrons available for sustaining the chain reaction. In LWRs, ϵ is slightly greater than one, with an approximate value of 1.03, indicating an enhancement due to fast fissions [67].

The above mentioned factors comprise of the k_∞ , which can be mathematically represented through equation 3.2, commonly referred to as the four-factor formula.

$$k_\infty = \eta \cdot \epsilon \cdot p \cdot f \quad (3.2)$$

Understanding these factors is essential for evaluating reactor performance and stability.

The Six-factor formula expands upon the Four-factor formula, enhancing the understanding of neutron behaviour in a finite reactor medium [63]. This formula incorporates two additional factors alongside the four previously identified factors:

1. **Fast non-leakage probability (P_f):** This is the probability that a fast neutron will remain inside the reactor and not escape until it slows down to thermal energy. It indicates the efficiency with which fast neutrons are contained within the reactor's geometry [68].
2. **Thermal non-leakage probability (P_t):** This indicates the probability that a thermal neutron is unlikely to leak out of the reactor and remain inside until it is absorbed. It reflects how effectively the reactor's geometry contains thermal neutrons [69].

The k_{eff} can be mathematically represented using the k_∞ along with two additional factors. These factors address neutron leakage during the thermalisation process and during diffusion. The first factor is the fast non-leakage probability, and the second is the thermal non-leakage probability. This relationship is encapsulated in Equation 3.3, commonly referred to as the Six-factor formula.

$$k_{\text{eff}} = k_\infty \cdot P_f \cdot P_t \quad (3.3)$$

This formula is a critical instrument for assessing reactor reactivity and ensuring safe and efficient operation.

3.1.2.1 k_∞ of a fuel assembly

k_∞ represents the infinite multiplication factor of a single fuel assembly under idealised conditions, which include:

- Assumes no neutron leakage.
- Depends exclusively on the fuel's composition and geometry.
- Independent of the reactor's physical size or core configuration [70].

3.1.2.2 k_{eff} of a full-core

k_{eff} represents the neutron balance within the reactor core, which includes:

- Accounts for neutron leakage and spatial effects.
- Influenced by core geometry, moderator distribution, fuel assembly arrangement, and burnup distribution [70].

3.1.3 Reactivity

Reactivity in nuclear engineering refers to the measure of how a nuclear reactor's neutron population changes over time. It is a crucial parameter that determines the departure from criticality and influences the overall behaviour of a nuclear reactor. Reactivity, denoted by the symbol ρ is defined by Equation 3.4 and is often expressed as per cent mille (pcm), equivalent to one-thousandth of a percent.

$$\rho = \frac{k_{\text{eff}} - 1}{k_{\text{eff}}} \quad (3.4)$$

where k_{eff} is the effective multiplication factor [62].

Reactivity changes resulting from temperature variations can be expressed mathematically as Equation 3.5.

$$\rho(T) = \rho_0 + \frac{\partial \rho}{\partial T}(T - T_0) \quad (3.5)$$

For this equation, $\rho(T)$ is approximated using a truncated Taylor series expansion about the reference temperature T_0 , while second-order and higher terms are neglected for simplicity.

Here, $\rho(T)$ denotes the reactivity as a function of temperature, and T_0 represents the reference temperature.

The reactivity of a reactor is influenced by factors that either increase or decrease the neutron population. These factors can be categorised into:

1. **Positive reactivity:** Anything that increases the neutron population and tends to make the reactor more reactive is considered positive reactivity. For example:
 - Withdrawing control rods from the reactor core causes the neutron population to increase because fewer neutrons are being absorbed. This leads to a rise in reactivity and, consequently, an increase in power output. This action constitutes an insertion of positive reactivity, as it makes the reactor more supercritical and enhances the fission chain reaction.
 - Increasing the enrichment level of the fuel can add positive reactivity. This is because enriched fuel has a higher likelihood of sustaining fission reactions.
2. **Negative reactivity:** Anything that decreases the neutron population and tends to make the reactor less reactive is considered negative reactivity. For example:
 - Inserting control rods made of materials that strongly absorb neutrons, thus reducing the overall neutron population.
 - Adding neutron-absorbing materials like boron to the reactor coolant.

The above processes are referred to as an insertion of negative reactivity, as they shifts the reactor toward a more subcritical state.

In reactor operation, the objective is to maintain the neutron multiplication factor, k , close to unity ($k \approx 1$), which indicates a stable and self-sustaining chain reaction. This requirement can be expressed mathematically by maintaining a small and positive reactor period, τ , which indicates the rate of power changes in the reactor. When the reactor is precisely critical ($k = 1$), the reactor period approaches infinity ($\tau \rightarrow \infty$), signifying a constant power output. However, if reactivity becomes increasingly positive and τ decreases toward a safety threshold of approximately 30 seconds, the reactor is approaching prompt supercriticality. This condition is deemed unsafe, prompting the Reactor Protection System (RPS) to initiate an automatic Safety Control Rod Axe Man (SCRAM) by rapidly inserting all control rods to terminate the reactor operations. Alternatively, if excessive negative reactivity is sustained, the reactor transitions to a subcritical state, effectively ceasing the chain reaction.

3.1.4 Nuclear data libraries

Nuclear data libraries in nuclear reactors are collections of data that represent the probability of specific nuclear interactions at a specific neutron energy. These interactions include neutron scattering, absorption, and fission. Nuclear data libraries are essential for accurately modelling neutron transport and predicting reactor behaviour [71]. Nuclear

data is typically presented as a function of neutron energy for various nuclides and nuclear reactions.

The accuracy of nuclear data libraries is crucial for the reliability of reactor simulations and safety assessments. Therefore, nuclear data is rigorously evaluated and benchmarked against experimental measurements to ensure their quality and validity. $S(\alpha,\beta)$ thermal scattering for light water was used for the moderator in this study; however, it was not applied to Oxygen in Uranium, as the corresponding nuclear data were unavailable. However, continuous efforts are made to improve and update nuclear data libraries. to incorporate new experimental data, advancements in nuclear theory, and refinements in computational methods.

Over the past two decades, the Evaluated Nuclear Data File (ENDF)/B series has evolved, improving the quality, coverage, and reliability of cross-section data critical for reactor physics and nuclear applications. The release of ENDF/B-VII.0 in 2008 marked a significant advancement, featuring expanded neutron cross sections and fission data [72]. Subsequently, ENDF/B-VII.1 was introduced in 2011, which provided broader nuclide coverage, covariance data, and enhanced evaluations for light nuclei and structural materials [73]. The 2018 release of ENDF/B-VIII.0 further refined intermediate and fast neutron data, aligning results more closely with experimental benchmarks [73]. The most recent release, ENDF/B-VIII.1 (2024) [74], includes targeted corrections and new evaluations for light elements, resulting in more accurate data for advanced modelling and benefiting from improved processing capabilities such as NJOY [75].

3.1.5 Neutron transport equation

The neutron transport equation describes the behaviour of neutrons in a medium, accounting for scattering, absorption, and fission processes. Refer to Equation 3.6 for the formal representation of the time-dependent neutron transport equation [76].

$$v \frac{\partial \phi(\mathbf{r}, E, t)}{\partial t} + \nabla \cdot (v \phi(\mathbf{r}, E, t)) = Q(\mathbf{r}, E, t) + \int_0^\infty \int_{4\pi} \Sigma_s(E' \rightarrow E) \phi(\mathbf{r}, E', t) d\Omega dE' \quad (3.6)$$

where:

- $\phi(\mathbf{r}, E, t)$ denotes the neutron flux,
- v represents the neutron speed,
- $Q(\mathbf{r}, E, t)$ is the source term,
- $\Sigma_s(E' \rightarrow E)$ corresponds to the scattering cross-section, and
- $d\Omega$ represents the solid angle.

The time-independent neutron transport equation models the steady-state population of free neutrons in a fissioning system. Under the assumption of equilibrium, where time dependence is negligible, the equation is expressed as Equation 3.7 [76].

$$\begin{aligned} \boldsymbol{\Omega} \cdot \nabla \phi(\mathbf{r}, E, \boldsymbol{\Omega}) + \Sigma_t(\mathbf{r}, E) \phi(\mathbf{r}, E, \boldsymbol{\Omega}) = & \int_{4\pi} \int_0^\infty \Sigma_s(\mathbf{r}, E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) \phi(\mathbf{r}, E', \boldsymbol{\Omega}') dE' d\boldsymbol{\Omega}' \\ & + \frac{\chi(E)}{4\pi} \int_0^\infty \nu \Sigma_f(\mathbf{r}, E') \phi(\mathbf{r}, E', \boldsymbol{\Omega}) dE', \end{aligned} \quad (3.7)$$

where:

- $\phi(\mathbf{r}, E, \boldsymbol{\Omega})$ is the angular neutron flux,
- $\Sigma_t(\mathbf{r}, E)$ is the total macroscopic cross-section,
- $\Sigma_s(\mathbf{r}, E' \rightarrow E, \boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega})$ is the differential scattering cross-section,
- ν is the average number of neutrons produced per fission,
- $\Sigma_f(\mathbf{r}, E')$ is the macroscopic fission cross-section, and
- $\chi(E)$ is the fission neutron energy spectrum.

Neutron transport codes implement a variety of algorithms to solve the neutron transport equation — whether by a deterministic numerical solver scheme or by a stochastic simulation in a Monte Carlo transport code. These include Monte Carlo methods, deterministic approaches such as the discrete ordinates method, diffusion theory, and hybrid methods. The selection of the algorithm significantly influences both computational efficiency and the accuracy of the solution.

The mathematical formulations employed in neutron transport algorithms differ based on the selected method, including the transport equation and the diffusion equation. The Serpent code utilises the Monte Carlo algorithm to address the neutron transport equation. It functions as a continuous-energy Monte Carlo neutron and photon transport code [77].

A key distinction between neutron diffusion solvers and neutron transport solvers is their treatment of the angular dependence of neutron flux. Diffusion theory simplifies the transport equation by assuming isotropic angular flux, thus eliminating the angular variable. This simplification leads to a reduction in computational complexity, making diffusion solvers, particularly nodal diffusion solvers, significantly faster than full transport solvers. However, for applications requiring high fidelity, where spatial and spectral heterogeneities are important, the diffusion approximation proves insufficient. In such scenarios, detailed transport solvers that account for angular dependence are essential [78]. The Monte Carlo code Serpent, utilised in this study, provides a high-fidelity neutron transport solution by simulating the stochastic behaviour of individual neutrons, thereby capturing the fine-scale physics necessary for accurate reactor analysis [79].

3.2 Thermal-hydraulics

The TH model is governed by three conservation equations: mass, momentum, and energy.

Mass conservation (Continuity equation) The mass conservation can be represented as Equation 3.8

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (3.8)$$

where:

- ρ is fluid density,
- $\mathbf{u}$ is the velocity vector.

Momentum Conservation (Navier-Stokes Equation) The momentum conservation can be represented as Equation 3.9

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} \right) = -\nabla p + \mu \nabla^2 \mathbf{u} + \mathbf{f} \quad (3.9)$$

where:

- p is pressure,
- μ is dynamic viscosity,
- $\mathbf{f}$ represents body forces.

Energy Conservation The energy conservation equation can be represented as Equation 3.10

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = k \nabla^2 T + Q \quad (3.10)$$

where:

- C_p is specific heat capacity,
- k is thermal conductivity,
- Q represents heat generation (from fission).

3.3 Epsilon and the epsilon equation

In this study, epsilon is employed to calculate the relative change in reactor state parameters between successive iterations. This approach is standard in numerical methods and reactor physics for evaluating variations in calculated parameters throughout iterations. The evaluation assists in determining whether the solution is converging, where changes become smaller over iterations, or diverging. In iterative methods such as those applied to solve neutron diffusion equations, epsilon functions as a convergence criterion. In N simulations, this metric is applicable for monitoring changes in neutron flux or reactor power as the simulation approaches a steady-state solution. This process ensures that results trend towards stability and convergence. Please see Equation 3.11 for the epsilon equation utilised.

$$\text{Power Epsilon} = \frac{|\text{Iteration 2 power} - \text{Iteration 1 power}|}{\text{Iteration 1 power}} \quad (3.11)$$

3.4 Validation and verification (V&V)

Differentiation between validation and verification in computational modelling is critical. Verification ensures that the input model, which includes geometry, material compositions, boundary conditions, and tally definitions, accurately reflects the physical system under analysis. This process verifies that the model has been constructed correctly in accordance with the specifications of the system being studied.

Validation involves demonstrating that the computational code and model yield accurate results by comparing calculated outputs to known reference data. Reference data may be sourced from benchmark problems published in the SAR or from high-quality experimental measurements obtained from calibrated instrumentation.

Thus, validation confirms that the model accurately represents the system, while verification ensures that the code effectively and reliably solves the model equations.

3.5 Design limits and criteria in pressurised water reactors

In the design of fuel for PWRs, strict adherence to specific safety and operational criteria is paramount to maintain the fuel license.

Total power peaking factor (F_Q): The total power peaking factor measures the variation in power distribution across the fuel assembly of a PWR. It is defined as the ratio of maximum local power to the average core power [80].

$$F_q = \frac{P_{\max}}{P_{\text{avg}}} \quad (3.12)$$

Nuclear Enthalpy Rise Hot Channel Factor ($F_{N\Delta H}$): Operation within the Nuclear Enthalpy Rise Hot Channel Factor ($F_{N\Delta H}$) limits, prevents DNB during accidents, which are critical from a DNB perspective [81]. This is represented by Equation 3.13

$$F_{N\Delta H} = \frac{\int_0^L q'_{\max}(z) dz}{\int_0^L q'_{\text{avg}}(z) dz} \quad (3.13)$$

where:

- $q'_{\max}(z)$ is the linear power along the fuel rod with the highest integrated power [kW/rod].
- $q'_{\text{avg}}(z)$ is the average rod power in the core [kW/rod].
- L represents the **active fuel length** of the fuel rod in the reactor core. It is the length over which the linear power distributions $q'_{\max}(z)$ and $q'_{\text{avg}}(z)$ are integrated.

Alternatively, it can also be expressed as Equation 3.14.

$$F_{N\Delta H} = \frac{\int_0^L q'_{\text{critical}}(z) dz}{\int_0^L q'_{\text{avg}}(z) dz} \quad (3.14)$$

where $q'_{\text{critical}}(z)$ is the linear power along the fuel rod on which the minimum departure from nucleate boiling ratio DNB occurs during Anticipated Operational Occurrence (AOO)s.

MTC: The moderator temperature coefficient (MTC) indicates the change in reactivity ρ per unit change ΔT in moderator temperature T in a nuclear reactor [82].

$$MTC = \frac{\Delta \rho}{\Delta T}$$

Doppler Coefficient (DC): The Doppler coefficient measures the reactivity change with respect to fuel temperature variations caused by the Doppler broadening effect [82].

$$DC = \frac{\Delta \rho}{\Delta T}$$

Departure from Nucleate Boiling Ratio (DNBR) Margin: The DNBR margin indicates the safety margin between local heat flux and critical heat flux, ensuring the prevention of nucleate boiling [82].

Shutdown Margin (SDM): Shutdown margin is a measure of the reactor's sub-criticality when control rods are fully inserted [82].

Rod internal pressure (RIP): This parameter specifies the maximum allowable internal pressure within the fuel rods of the reactor [80].

Core Critical Boron Concentration (CBC): This represents the concentration of boron in the reactor core needed to achieve criticality [80]. A design limit is imposed on CBC to guarantee the MTC stays negative (or non-positive) at all power levels, ensuring that temperature increases do not lead to uncontrolled power escalation and maintaining safe, stable reactor conditions [83].

Fuel Center-line Temperature: This limit ensures that the temperature at the centre-line of the fuel remains below the melting temperature range [80].

Clad Outside Surface Temperature: This parameter specifies the maximum allowable temperature on the outer surface of the fuel cladding [80]. Exceeding this temperature poses safety risks in nuclear reactors. In commercial reactors utilising Zircalloy as the cladding material, zirconium oxidation can occur, leading to the formation of zirconium dioxide and the release of Hydrogen gas. Accumulated Hydrogen presents an explosion risk, evidenced by the Fukushima incident [84]. Additionally, excessive temperatures can lead to the melting of cladding, potentially resulting in a core meltdown scenario and radioactive release similar to that of Fukushima.

While these design parameters define the operational framework of a PWR, it is the design limits that ensure the reactor operates safely within this framework under all expected conditions. PWR fuel must satisfy a range of design limits and criteria as follows:

- F_Q : ≤ 2.60 including uncertainties ([85])
- MTC: ≤ 0 pcm/K ([86])
- DC: ≤ 0 pcm/K ([86])
- DNBR margin: ≥ 15 % ([85])
- SDM: ≥ 1.6 % $\Delta\rho$ or ≥ 1300 pcm ([85])
- RIP: ≤ 2600 psia ([86])
- CBC: ≤ 1780 ppm ([86])
- Fuel centre-line temperature: Adequate margin must ensure operation below the melting temperature range of $2600\pm 2800^\circ\text{C}$ ([86])
- Clad outside surface temperature: ≤ 673.15 K ([86])

The criteria are critical for ensuring the safe and efficient operation of PWRs. They regulate factors such as thermal performance, safety margins, and core criticality.

3.6 Conclusion

This theory chapter highlights the importance of key N parameters, including reactivity and k_{eff} , in relation to reactor criticality and safe operation, emphasising the need for precise reactivity control. The selection of appropriate neutron transport algorithms and coupling interfaces is discussed as critical for enhancing computational efficiency and accuracy. Additionally, this chapter examines various TH equations that are fundamental for the understanding of the TH model. Validation and verification processes are outlined as essential for ensuring the reliability of N and TH codes, while effective utilisation of computational resources contributes to accurate simulations. Compliance with safety standards and regulatory requirements is considered vital for maintaining reactor integrity.

The theories and equations presented in this chapter facilitate coupling and improve comprehension of reactor behaviour, aligning with the objectives of the study.

The next chapter will examine the methodology employed in the coupling process.

Chapter 4

Methodology

This chapter details the methodology used to couple N and TH through High-Performance Computing (HPC) platforms. The justification for selecting these specific computer software tools is provided, along with an explanation of the rationale for these choices. The reactor geometry of NAPS, highlighting modifications to previous models that utilised the LOPAR fuel assembly for improved representation of the latest fuel assembly, RFA-2, will be addressed. Additionally, the configurations of the various N models are reviewed and altered, along with the verification and validation processes applied to each model.

4.1 Tools and codes

Computational tools for N and TH play a crucial role in nuclear reactor simulations, taking into account the complexity of reactor systems, safety standards, and optimisation objectives associated with reactor design and operation. Achieving coupling between N and TH using Serpent (for N) and Flownex (for TH) can improve the accuracy of pin-level, fuel assembly, and full-core simulations. This coupling is important because N reactions (fission, absorption, scattering) and TH conditions (heat transfer, fluid flow) are interdependent, and their interaction affects reactor behaviour.

4.1.1 Neutronics code: Serpent

Serpent is a Monte Carlo particle transport code developed by the Finnish VTT Technical Research Centre, used for simulating neutron interactions in nuclear reactors. Its versatility and accuracy make it a widely used tool among nuclear engineers [77].

Key features of Serpent include its use of the Monte Carlo technique [77], which simulates neutron interactions such as scattering, absorption, and fission across reactor geometries. This stochastic method is supported by cross-section libraries, allowing for neutron transport simulations. Users can model geometries in 2D and 3D, accommodating various fuel

types and structural components [77]. Additionally, Serpent supports isotope and material handling [87], along with burnup calculations to evaluate reactor performance over time [88]. Its parallel processing capabilities allow for efficient use of multiple CPU cores, reducing simulation times for large-scale models. Serpent benefits from a user community, enhancing its utility through shared resources and ongoing development.

The Serpent Monte Carlo code is recognised for its application in nuclear reactor studies, demonstrating its utility in N calculations. Notable uses include:

- **3D full-core simulations:** Used in designing 3D reactor cores, such as the European Sodium Fast Reactor (ESFR), Serpent supports safety evaluations by generating compatible group constants for deterministic methods [89].
- **Coupled multi-physics applications:** Integrated into the Kraken framework¹, Serpent facilitates complex simulations that include N, TH, and fuel behaviour [90].
- **Burnup calculations:** It enables tracking of nuclide concentrations, aiding fuel cycle assessments and spent fuel analysis [91].
- **Validation of deterministic codes:** Frequently used to validate deterministic transport codes, ensuring accuracy in criticality safety and fuel cycle studies [91].
- **Research reactor modelling:** Its flexibility allows for modelling unique geometries in research reactors [92].
- **Educational use:** With extensive global use in academia, Serpent supports research and thesis work in nuclear engineering [93].

Overall, Serpent is a significant tool in nuclear reactor physics, used in both academic and industrial applications.

4.1.2 Thermal-hydraulics code: Flownex

Flownex® Simulation Environment (SE), developed in Potchefstroom, South Africa, is a 1D thermal-fluid system simulation software such as RELAP or TRACE, that has been developing since 1986. The latest version, Flownex SE 2025 Release 2 (Version 9.0.1), was released in April 2025. This version introduces enhancements such as adaptive timestep solvers, psychrometric capabilities, Functional Mock-up Interface (FMI) support, and machine learning-based reduced order models. The updates in the 2024 and 2025 releases focus on automation, increased accuracy, improved project management, and enhancements to user experience. Flownex has transitioned from a mining network solver to a recognised, nuclear-accredited simulation environment, adapting its features to address the evolving requirements of engineering simulation [94].

¹Kraken is a computational framework that couples neutron transport solvers like Serpent with thermal-hydraulics and fuel performance codes to enable high-fidelity, multiphysics reactor simulations.

Flownex is used for analysing mechanisms such as hydraulics, pneumatics, and heat-exchange systems. Equipped with a Graphic User Interface (GUI), Flownex enables engineers to create models involving components such as pipes, valves, and heat exchangers. Users can specify fluid properties, boundary conditions, and operating parameters to simulate different scenarios, aiding in the evaluation of system performance and design optimisation prior to physical prototyping [95]. Flownex features a Distribution Heat Source (DHS) element that supports the incorporation of a distributed heat source such as nuclear fuel. DHS facilitates the specification of heat input along the length of a component, thereby enhancing the accuracy of simulations concerning heat absorption or release through material layers in the direction of heat transfer. This includes defining the overall heat fraction, the heat fraction of the flow, and the heat distribution across layers, which improves the precision of thermal behaviour modelling. Additionally, a local specification option for heat input associated with DHS has been integrated [96]. This enhancement improves thermal analysis by providing a more accurate representation of heat distribution within a system, thereby ensuring that simulations are closely aligned with actual conditions.

Utilising Serpent and Flownex for coupled N and TH simulations enhances the precision of reactor analysis, specifically for pin, fuel assembly, and full-core simulations [97]. This coupling provides data on reactor performance, supports design optimisation, and improves reactor operational safety by accurately predicting interactions between N and TH phenomena [87]. The current study builds on earlier research conducted by Mashilangako [98], which utilised Serpent and Flownex in coupling Koeberg PWR for N and TH analysis. The present research aims to extend this work by implementing a pin-by-pin approach for fuel assembly coupling.

In this study, Serpent and Flownex were executed on separate computers, with results transferred between the two systems. Serpent operates on a Linux platform, which is tailored for Monte Carlo neutron transport simulations that require effective parallel processing capabilities provided by Linux clusters. Flownex operates on Windows, functioning as commercial TH systems simulation software primarily intended for engineering applications in industrial environments. Coupling will be performed on a server to ensure continuous operation, thereby reducing the risk of interruptions typically associated with personal computers, which may experience frequent power-downs. Server environments are equipped to support job scheduling and parallel execution, which are essential for the efficient management of extended Serpent simulations.

4.1.3 Justification of selection of computational tools (codes)

Flownex and Serpent are recognised tools in nuclear reactor design and analysis, noted for their complementary capabilities in TH and N modelling. Here are the key reasons for their preference:

- Integrated system modelling: Flownex provides a comprehensive environment for simulating fluid mechanics, heat transfer, and control systems in nuclear plants. It allows for total plant modelling, integrating reactor dynamics with balance-of-plant performance and control logic in a single platform. This holistic approach facilitates better understanding and optimisation of system-level performance [99].
- Accurate N calculations: Serpent excels in performing detailed N calculations, including eigenvalue and burnup analyses. This capability is essential for evaluating reactor behaviour under various operating conditions. When coupled with Flownex, Serpent enhances the accuracy of TH simulations by providing precise reactivity feedback and core power distribution profiles [100].
- Efficiency in design and safety analysis: Both tools streamline the design process, allowing for rapid simulations that support technical feasibility studies, accident scenario investigations, and optimisation studies. Flownex's fast-solving speed enables quick decision-making during the design phase, while Serpent's detailed modelling supports rigorous safety assessments [101].
- Regulatory compliance: Flownex offers features that assist in the demonstration of meeting regulatory requirements, including a Certificate of Compliance and a Verification and Validation (V&V) package. This is crucial for nuclear projects where adherence to safety standards is paramount [99].
- Versatility and compatibility: The ability to integrate with other software tools (like MATLAB and Ansys) allows for enhanced functionality, making these tools adaptable to various project needs. This versatility is particularly beneficial in complex reactor designs where multiple analyses are required [102].

In summary, the combination of Flownex's well-documented [103] TH capabilities with Serpent's high-fidelity N capabilities makes them a powerful duo for nuclear reactor analysis, ensuring robust design, safety compliance, and efficient project execution.

4.2 Coupling mechanisms

This section examines the mechanisms utilised in coupling N and TH, as well as the interaction and data exchange between the Serpent and Flownex solvers in this study. For the coolant, a cool.ifc input file will be generated to extract ten axial values of average coolant temperature and density from Flownex. For the fuel, a fuel.ifc input file will be created to supply Serpent with five radial fuel temperatures at each of the ten axial positions. This discretisation is intended to capture the spatial variation of N and TH parameters with sufficient resolution, ensuring accurate iterative feedback between the solvers.

4.2.1 Neutronics to thermal-hydraulics coupling

The power distribution derived from N calculations, extracted from the Serpent det.0 file as 10 axial values, serves as the heat source for TH simulations, accounting for axial variation in the distribution.

4.2.2 Thermal-hydraulics to neutronics

Temperature-dependent cross-sections are updated based on TH results, specifically of the fuel and coolant temperatures. This can be represented as:

$$\sigma(T) = f(T)$$

Where:

- $f(T)$: a function that describes the variation of cross-sections with temperature.

TH to N coupling continually updates water density as it changes with coolant temperature, feeding those values into the N module to update the moderation and reactivity. The process is iterative and often applies interpolation formulas for cross-section update by water density [47].

This can be expressed mathematically as a function of temperature with pressure held constant (often near operating pressure):

$$\rho = \rho_0 \times (1 - \beta \times (T - T_0))$$

where:

- ρ_0 = reference water density at temperature T_0 (e.g., 1000 kg/m³ at 20°C)
- β = volumetric thermal expansion coefficient of water (approximately 0.0003 to 0.0004 per °C)
- T = current water temperature
- T_0 = reference temperature

4.2.3 Iterative coupling process

As discussed in Section 2.3.2, various types of coupling exist. This study utilises the external serial integration coupling strategy method, which includes:

1. Performing N calculation to obtain power distribution.
2. Updating TH parameters based on power distribution.
3. Adjusting material properties and cross-sections based on temperature and density from TH.
4. Repeating until results stabilise.

4.2.4 Conclusion

The mathematical modelling of the coupling between N and TH necessitates the integration of various physical principles and equations to address complex interactions. By employing these models, engineers can achieve high-fidelity simulations that enhance reactor safety and performance analysis.

4.3 Reactor geometry

This section examines the NAPS reactor geometry to ensure accurate results in the coupling process.

4.3.1 Core configuration

The NAPS's core configuration is critical for its operation and safety. Based on the information from the 2020 SAR [1], here is an overview of the core configuration, specifically focusing on the number of fuel assemblies and their arrangement:

1. Total number of fuel assemblies:
 - The NAPS core consists of 157 fuel assemblies arranged in a 15×15 Cartesian grid inside the core. This configuration is typical for Westinghouse-designed 3-loop PWRs.
2. Fuel assembly arrangement:
 - The fuel rods are arranged in a 17x17 lattice pattern, which includes:
 - 264 fuel rods per fuel assembly.
 - 24 control rod guide tubes that allow for the insertion and removal of control rods.
 - 1 central instrument tube for monitoring purposes.

Figure 4.1 shows the internal layout of the NAPS fuel assembly, including fuel rods, guide thimbles, control rod cluster locations, and instrumentation sheaths..

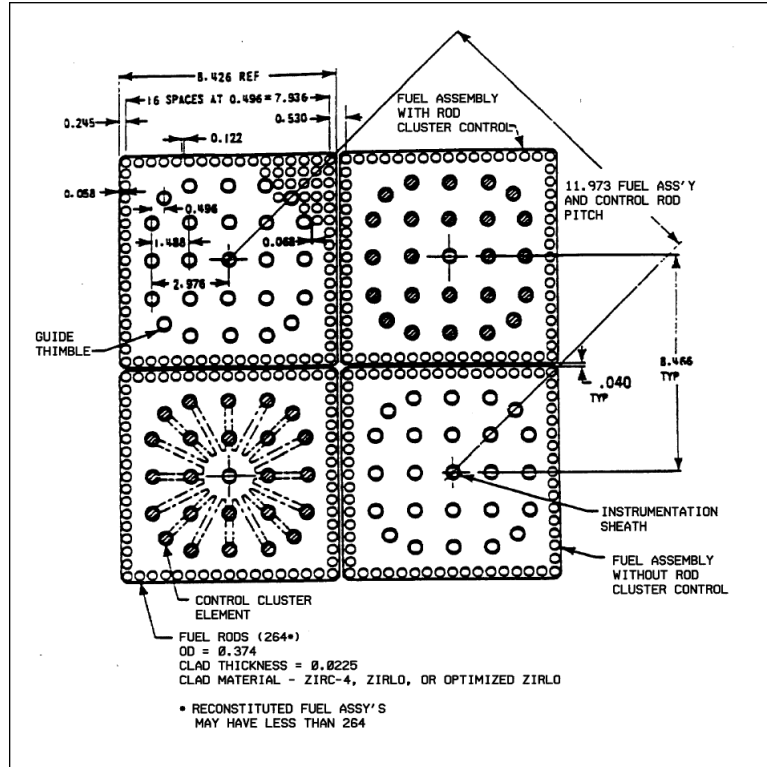


Figure 4.1: Schematic of the NAPS PWR fuel assembly arrangement showing fuel rods, guide thimbles, control cluster locations, and instrumentation sheaths[1].

3. Symmetry and batch loading:

- The loading pattern for the core is approximately eighth-core symmetric, meaning that similar fuel assemblies are grouped together to optimise performance and manage reactivity effectively.
- The core includes three fuel batches with enrichments- 2.1 wt %, 2.6 wt % and 3.1 wt %, which are loaded in a symmetric grouping to maintain balance and efficiency. Figure 4.2 presents a full-core loading map example where each block represents a fuel assembly made up of multiple pins.

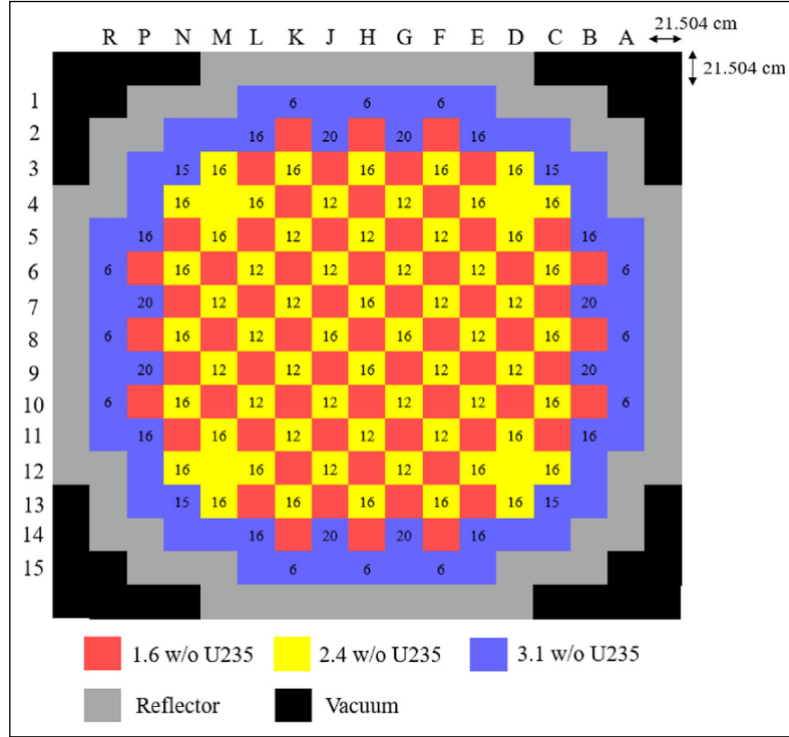


Figure 4.2: Full-core loading map example [2]

The core configuration at NAPS comprises 157 fuel assemblies arranged in a 15×15 Cartesian grid. Each fuel assembly features a 17×17 lattice that incorporates both fuel and guide rods. Please see Figure 4.3 for full-core configuration.

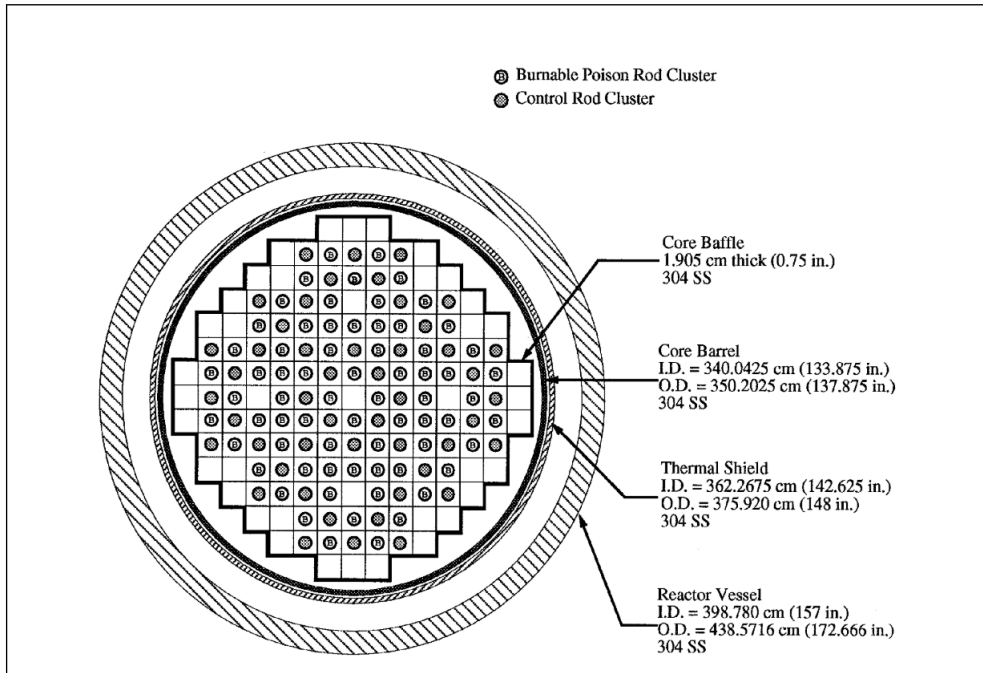


Figure 4.3: North Anna unit 1 cycle 5 core configuration [3]

4.4 Comparison of RFA-2 and LOPAR designs

This study will model the Westinghouse the RFA-2 fuel assembly, identified as the most recent fuel assembly design approved for use in the Koeberg power station [104]. This section will compare the RFA-2 fuel assembly design parameters with the previously used LOPAR model.

4.4.1 Design differences

The NAPS utilises fuel assemblies to improve performance and safety. The following is a comparison between the RFA-2 fuel assembly and the outdated LOPAR design:

- **Material improvements:**
 - The RFA-2 design utilises Zirlo cladding, offering better corrosion resistance and structural integrity than the Zircalloy used in LOPAR.
- **Structural enhancements:**
 - RFA-2 features an optimised debris filter and standardised bottom nozzle, enhancing coolant flow and reducing debris-related issues.
- **Grid design:**
 - The RFA-2 includes advanced grid support, providing improved fuel rod stability and reducing vibration compared to the LOPAR design. RFA-2 fuel assembly uses Zr-alloy for most grids – absorbs less neutrons and lower impact on axial power distribution, compared to nickel alloy (inconel) fuel pin support grids.
- **Geometric adjustments:**
 - The slightly altered fuel rod length in RFA-2 contributes to better neutron moderation and heat transfer.
- **Performance and safety:**
 - These enhancements allow the RFA-2 fuel assembly to achieve higher burnup, improving efficiency and operational safety.

The RFA-2 design shows advancements compared to the LOPAR fuel assembly. see Table 4.1.

Parameter	LOPAR Design	RFA-2 Design
Fuel assembly length	405.803 cm	406.337 cm (ZIRLO)
Fuel rod length	384.962 cm	388.112 cm (Optimised ZIRLO)
Fuel assembly pitch	21.402 cm	21.402 cm
Fuel rod pitch	1.260 cm	1.260 cm
Number of fuel rods/assembly	264	264
Number of guide thimbles/assembly	24	24
Fuel tube material	Zircaloy-4	Optimised ZIRLO
Fuel rod clad o.d.	0.950 cm	0.950 cm
Fuel rod clad thickness	0.057 cm	0.057 cm
Fuel/clad gap	0.017 cm	0.017 cm
Fuel pellet diameter	0.819 cm	0.819 cm
Fuel pellet length	1.346 cm	0.982 cm
Guide thimble material	Zircaloy-4	Optimised ZIRLO
Guide thimble o.d.	1.224 cm	1.224 cm.
Structural material - Six inner grids	Inconel	ZIRLO
Structural material - Two end grids	Inconel	Inconel
Grid inner strap Thickness	0.027 cm (Inconel grid)	0.046 cm (ZIRLO grid)
Grid outer strap thickness	0.043 cm (Inconel grid)	0.066 cm (ZIRLO grid)
Grid support for fuel rods	6 Points, 2 Springs, 4 Dimples	6 Points, 2 Springs, 4 Points (P-grid)
Grid height	3.358 cm (mid Grids)	3.810 cm (mid Grids)
Grid fabrication method	Brazed joining	Laser welded interlocking
Grid/Guide thimble attachment	Thimbles and sleeves	Laser prewelded into grid straps
Bottom nozzle	Reconstitutable	Advanced Debris Filter Bottom Nozzle

Table 4.1: Comparison of 17 x 17 LOPAR fuel assembly and RFA-2 fuel assembly dimensions [1]

4.4.2 Significance

The accurate modelling of the geometry of structures and components is essential in nuclear reactor analysis, affecting N (neutron behaviour) and TH (heat transfer and fluid dynamics). The design and arrangement of fuel assemblies, control rods, and coolant channels influence reactor performance and safety margins.

N and Geometry

- **Fuel assemblies:** Placement affects neutron flux and reactivity.
- **Moderator and reflector:** Impact neutron energy and reactivity.
- **Control rods:** Geometry controls power output and emergency shutdown capabilities.

Impact on Neutron behaviour

- **Flux and leakage:** Geometry affects neutron travel and leakage.

- **Fuel burnup:** Arrangement ensures even fuel depletion, enhancing efficiency.

TH and Geometry

- **Coolant flow:** Channel design impacts heat transfer efficiency.
- **Core shape:** Affects heat removal, especially during transients.

Coupling of N and TH Geometry influences the interaction between N and TH through feedback mechanisms, affecting neutron flux, temperature distribution, and the total reactor power.

Importance for modelling and Safety Accurate geometric modelling is essential for reactor simulation and safety analysis, enhancing fuel efficiency and safety.

4.4.3 ZIRLO composition

In this model, ZIRLO has been chosen as the cladding material due to its enhanced corrosion resistance and improved high-temperature performance compared to Zircaloy. ZIRLO, a zirconium-based alloy incorporating niobium, tin, and iron, marks a significant advancement in cladding materials, moving from traditional Zircaloy (Zr-Sn) to more sophisticated Zr-Nb-Fe compositions. This evolution aims to improve fuel reliability under more rigorous operating conditions. Subsequent developments include Optimized ZIRLO, AXIOM, and M5 cladding, all designed to minimise corrosion and Hydrogen absorption by reducing or eliminating tin content while optimising the proportions of niobium and iron. The composition of ZIRLO, as calculated in Table D.1 and utilised in the model, is detailed in Table 4.2.

Element	Atom Fraction
8016.03c	1.3995E-03
8017.03c	5.3200E-07
24050.03c	2.0422E-06
24052.03c	3.9381E-05
24053.03c	4.4655E-06
24054.03c	1.1115E-06
26054.03c	5.8450E-05
26056.03c	9.1754E-04
26057.03c	2.1190E-05
26058.03c	2.8200E-06
40090.03c	5.0295E-01
40091.03c	1.0968E-01
40092.03c	1.6765E-01
40094.03c	1.6990E-01
40096.03c	2.7371E-02
41093.03c	1.0000E-02
50112.03c	9.7000E-05
50114.03c	6.6000E-05
50115.03c	3.4000E-05
50116.03c	1.4540E-03
50117.03c	7.6800E-04
50118.03c	2.4220E-03
50119.03c	8.5900E-04
50120.03c	3.2580E-03
50122.03c	4.6300E-04
50124.03c	5.7900E-04

Table 4.2: ZIRLO composition: Elements and their atom fractions

Detailed ZIRLO material properties are provided in Appendix E.

4.5 Model setup

This section outlines the steps for setting up the N and TH models for the study.

4.5.1 Neutronics model setup

To verify and validate a N model for this dissertation, access was granted to two existing NAPS N models developed by North-West University (NWU) nuclear engineering students. The first Serpent model, created by Ringane [105], using NWURCS, while the second Serpent model was developed ab initio by Mphofu [106].

The task involved comparing these two models to each other and to the latest version of the NAPS SAR. To ensure that the models accurately represented the updated SAR, several modifications were implemented.

4.5.1.1 Steps and procedure for the full-core

1. Software setup and configuration

To effectively run the Serpent N software for the thesis, follow these steps for installation and access on the HPC at NWU:

(a) HPC access application:

- Begin by applying for access to the HPC through the online form.
- Upon approval, login credentials will be provided by the system administrators, typically using the student number for both username and password.

(b) Connecting to Yamato cluster:

- Use the IP address 143.160.84.125 to connect to the Yamato cluster where Serpent will be executed.
- Download and install MobaXterm for interfacing with the HPC.

(c) VPN Setup for off-campus access:

- Ensure a VPN connection to NWU if accessing from off-campus.

(d) IT support for setup:

- Contact the IT support desk for assistance with installation, providing necessary identification details.

2. Model configuration

N model setup for NWURCS

The NWURCS code suite was used to develop the Serpent N calculation model of the NAPS reactor, based on the SAR RFA-2 fuel assembly specifications. The process involved:

- (a) **Input file modification:** Update the `input.mat` file to reflect material compositions and densities from the 2020 SAR report.
- (b) **Serpent input generation:** Generate and execute a Serpent input file, aligning materials and model dimensions with updated analysis.

- (c) **Operational adjustments:** Run materials at 300 K and 2940 MWt operational power.
- (d) **Cross-section library update:** Update the cross-section library from JEFF-2 to ENDF7.
- (e) **Structural enhancements:** Add upper and lower reflectors, thermal shields, a barrel, and baffles.
- (f) **Dimensional and fuel rod adjustments:** Update the fuel assembly, fuel rod, and fuel pellet lengths to match safety analysis specifications.

N Model Setup for Manual Model

The manual model aimed to represent RFA-2 fuel assembly specifications from the NAPS SAR. The setup included:

- **Skill development:** Utilise Serpent Wiki tutorials and convert Octave codes to MATLAB.
- **Model alterations:** Change dimensions to switch to the RFA-2 fuel assembly.
- **Material verification:** Verify material compositions and densities, updating to ZIRLO cladding.
- **Materials consistency:** Mirror NWURCS material atomic compositions for consistency.

These modifications ensure that both the NWURCS and manual models accurately represent the specified parameters and conditions.

The procedure for HPC access, software installation, and model setup is depicted in Figure 4.4, outlining the sequential steps necessary for successful configuration.

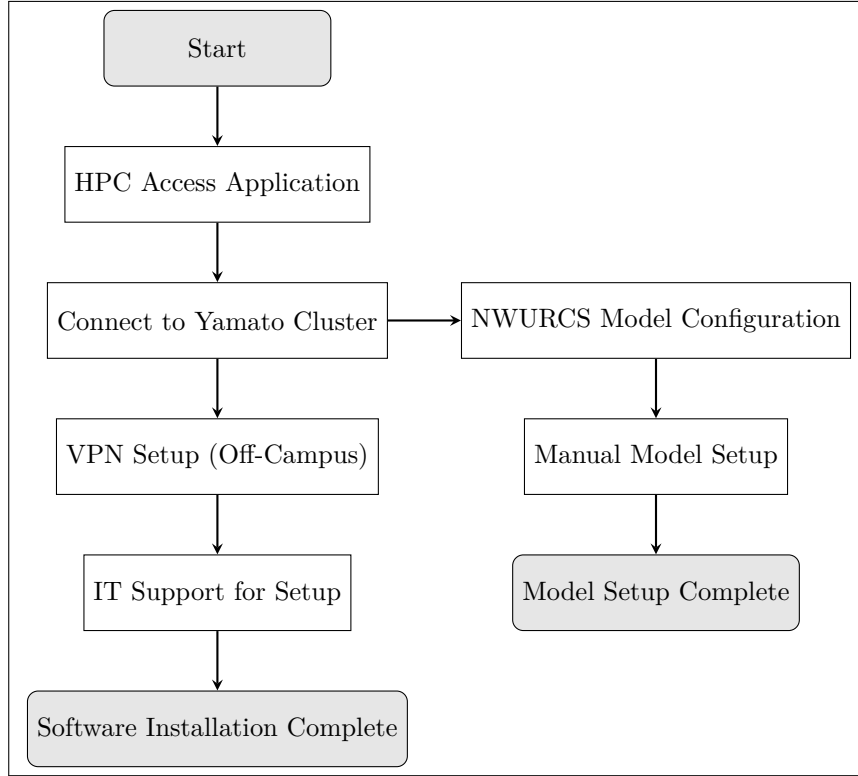
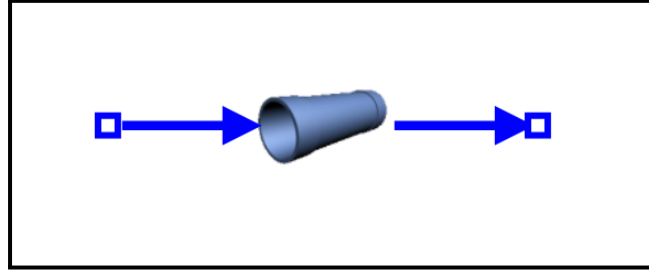


Figure 4.4: Workflow for High-Performance Computing access, software installation, and model setup

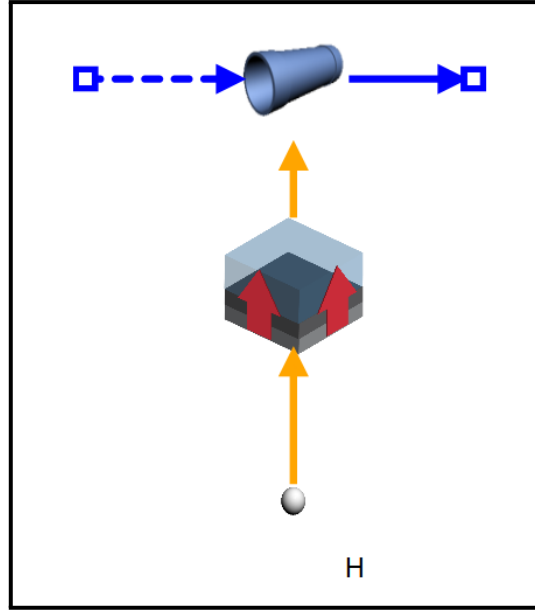
The N model in this study does not include soluble boron concentration or its reactivity effects. This simplification was made to isolate the impact of moderator temperature feedback on the N/TH coupling without the additional complexity introduced by chemical reactivity control. Excluding boron allows the analysis to focus solely on temperature- and density-driven reactivity changes, while acknowledging that in borated systems, soluble boron would contribute a competing effect that could influence overall reactivity behaviour.

4.5.2 Thermal-hydraulics model setup

The TH model was amended from a previous study [98] using Flownex software version 8.16.0.5519. For this study, the coolant is modelled in Flownex as a vertical pipe with upward flow. The fuel is represented as a distributed heat source, incorporating the fuel gap and cladding layers, and transfers heat to the pipe through specified heat transfer areas. Each fuel pin channel is modelled as a rod-centred pipe with no cross-flow between channels. Refer to Figure 4.5 for the representations of the fuel pin channel and guide tube channel in Flownex.



(a) Guide tube channel



(b) Fuel pin channel

Figure 4.5: Flownex fuel pin and guide tube channels

The fuel assembly model in Flownex was defined using boundary conditions obtained from the SAR. The inlet temperature was set to 561.87 K. The mass flow rate, calculated as the core thermal flow from the SAR divided by 157 assemblies, was 111.87 kg/s. The outlet pressure was specified as 15,322.22 kPa, determined by subtracting the core pressure drop from the system pressure. The model dimensions were modified to align with the SAR geometry parameters. The modifications included the following:

- **Fuel pin channel:** The wetted perimeter and flow area were adjusted, and the length of the channel was increased. Core pressure drop were updated according to the SAR [1], and the surface roughness was updated according to a study by Lee [107]. Configuration of thickness in both element direction and the cross direction, as well as the area of UO_2 , the gap, and cladding was completed.
- **Guide tube channel:** Since the guide tube channel was not implemented in previous models, it was introduced in this study with defined wetted perimeter, flow area, and channel length. The wetted perimeter was calculated as the sum of the outer and inner perimeters of the guide tube, as coolant flows along both surfaces.

- **Material properties:**

Parameter	Value	Unit
Fuel Pin Channel:		
Wetted perimeter	2.9843	cm
Flow area	0.8784	cm ²
Fuel rod length	388.112	cm
Average rise	39	K
Core pressure drop	190.9848	Pa
Surface roughness	1.61	μm (micrometer)
Guide Tube Channel:		
Wetted perimeter	15.0656	cm
Flow area	1.2045	cm ²
Material Properties:		
UO₂:		
Thickness in element direction (fuel radius)	0.4096	cm
Thickness in cross direction (axial height of fuel)	388.112	cm
Area	998.7804	cm ²
Gap:		
Thickness in element direction (gap thickness)	0.0083	cm
Thickness in cross direction (axial height of fuel)	388.112	cm
Area	1018.9109	cm ²
Cladding:		
Thickness in element direction (cladding thickness)	0.0572	cm
Thickness in cross direction (axial height of fuel)	388.112	cm
Area	1158.2756	cm ²

Table 4.3: Input parameters for fuel pin and guide tube channels used in the Flownex model [1]

Following the implementation of the changes in Table 4.3, a steady-state simulation was conducted without notable errors.

4.5.2.1 Challenges and solutions

The initial setup utilised an older version of Flownex (version 8.16.0.5222). Challenges with outdated features and limited updates were observed. To resolve these issues, the system was updated to version 8.16.0.5519. This updated version included improved features and debugging enhancements, facilitating a more efficient setup process.

4.6 Neutronics model verification

The verification and validation process is critical for ensuring the accuracy and reliability of N models and their coupling mechanisms. Before this process, the initial models, which serve as foundational representations of the systems, are defined and analysed. The figures of these initial models, presented in Figure 4.6, provide a baseline for comparison.

This section outlines a method for modifying the verification steps into a structured format. It includes the creation of a flowchart and a table to communicate the results of this process effectively. Through systematic updates and adjustments, the models are refined to align with the RFA-2 fuel assembly specifications, operational conditions, and enrichment levels as detailed in the safety analysis report.

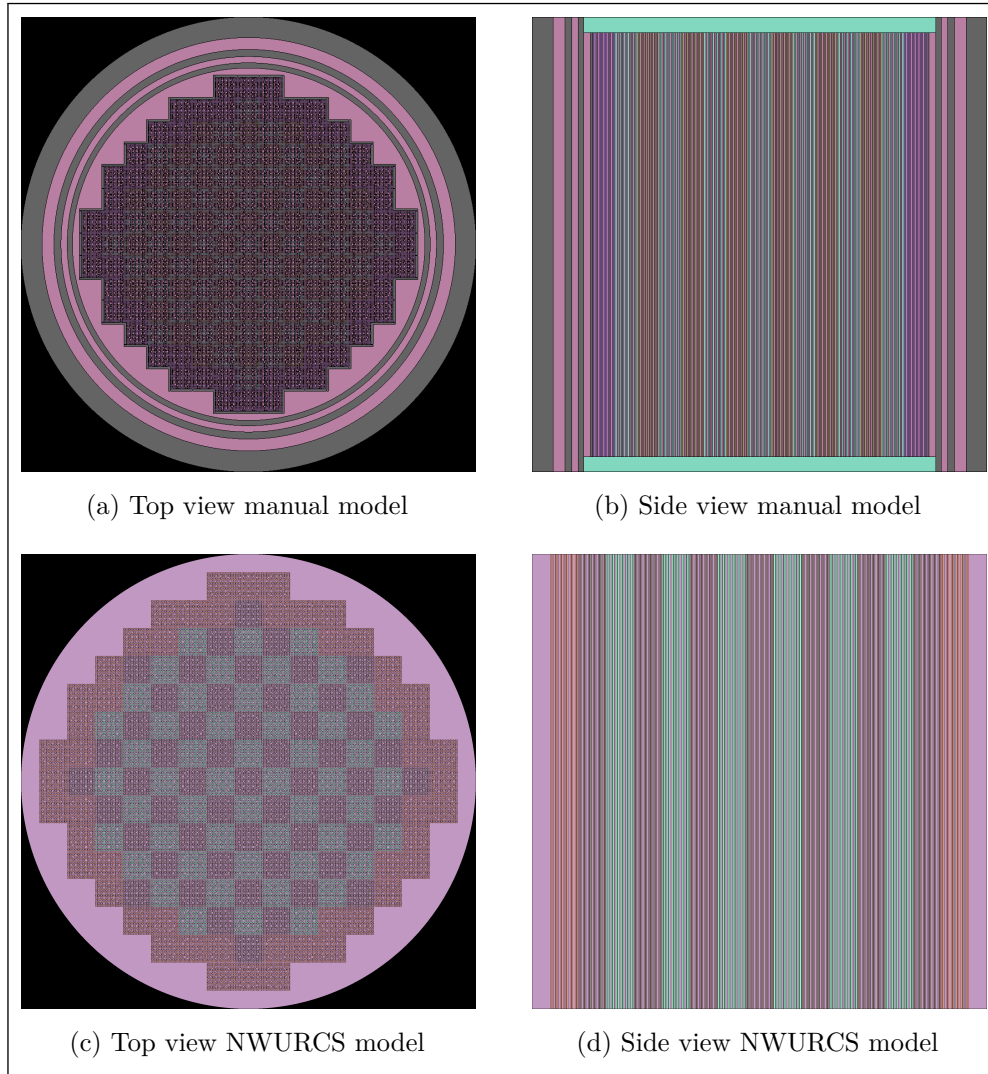


Figure 4.6: Comparison of top and side views of the manual and NWURCS full-core models

Following the visual comparison of the manual and NWURCS models in Figure 4.6, a verification and validation process is conducted. This process is necessary to confirm that the models meet the specified requirements and perform accurately under defined conditions. The following steps outline the modifications and checks implemented to attain alignment with the RFA-2 fuel assembly detailed in the safety analysis report:

1. **Fuel assembly update:** Modify both models to incorporate the RFA-2 fuel assembly specifications.
2. **Operational conditions:** Run simulations for materials at a temperature of 300 K and operational power of 2940 MWt.
3. **Cross-section libraries:** Utilise the ENDF/B-7.1 cross-section data (2011) for both models.
4. **NWURCS enhancements:** Assign and incorporate additional components in

NWURCS, such as a barrel, baffles, Reactor Pressure Vessel (RPV), thermal shields, and reflectors. See Table 4.4 for the component dimensions.

Component	Dimension (cm)
Core baffle	1.905
Core barrel:	
Inside diameter	340.0425
Outside diameter	350.2025
Thermal shield:	
Inside diameter	362.2675
Outside diameter	375.92
Reactor vessel:	
Inside diameter	398.78
Outside diameter	438.5716
Top/bottom reflector: 50% H O (0 ppm B), 50% SS-304 (wt%) [3]	25

Table 4.4: Reactor component dimensions [3]

5. **Fuel composition bug:** A bug was identified after aligning the NWURCS Uranium fuel composition with the manual model specifications. The incorporation of U-234 abundance from the manual model into the NWURCS model, which had initially excluded U-234 due to its minimal presence, resulted in instances where the density of U-234 exceeded that of U-235 during simulations. This anomaly led to a decrease in the k_{eff} value of Zirlo within the NWURCS model.
6. **Fuel rod adjustments:** Update the NWURCS fuel control rod inside radius to align with the safety analysis report, i.e. the NAPS SAR.
7. **Fuel enrichment discrepancy:** Identified and that the manual model's fuel enrichment region 2.6 % must be 3.1 % and the 3.1 % region must be 2.6 % to match the NWURCS model and the NAPS SAR.
8. **Symmetry and enrichment correction:** Adjust the manual model to ensure symmetry and update its fuel enrichment to reflect the NAPS SAR.
9. **Population settings:** For both full-core models, the simulation population settings were configured as "100000 300 150", meaning 100,000 neutron histories per cycle, 300 active cycles, and 150 inactive (discarded) cycles. These inactive cycles are excluded from tallies to allow the volume-distributed fission neutron source to settle

to the fundamental mode before statistical sampling begins, which is essential for convergence in eigenvalue calculations.

Refer to Figure 4.7 for the flowchart utilised in the verification of the N model.

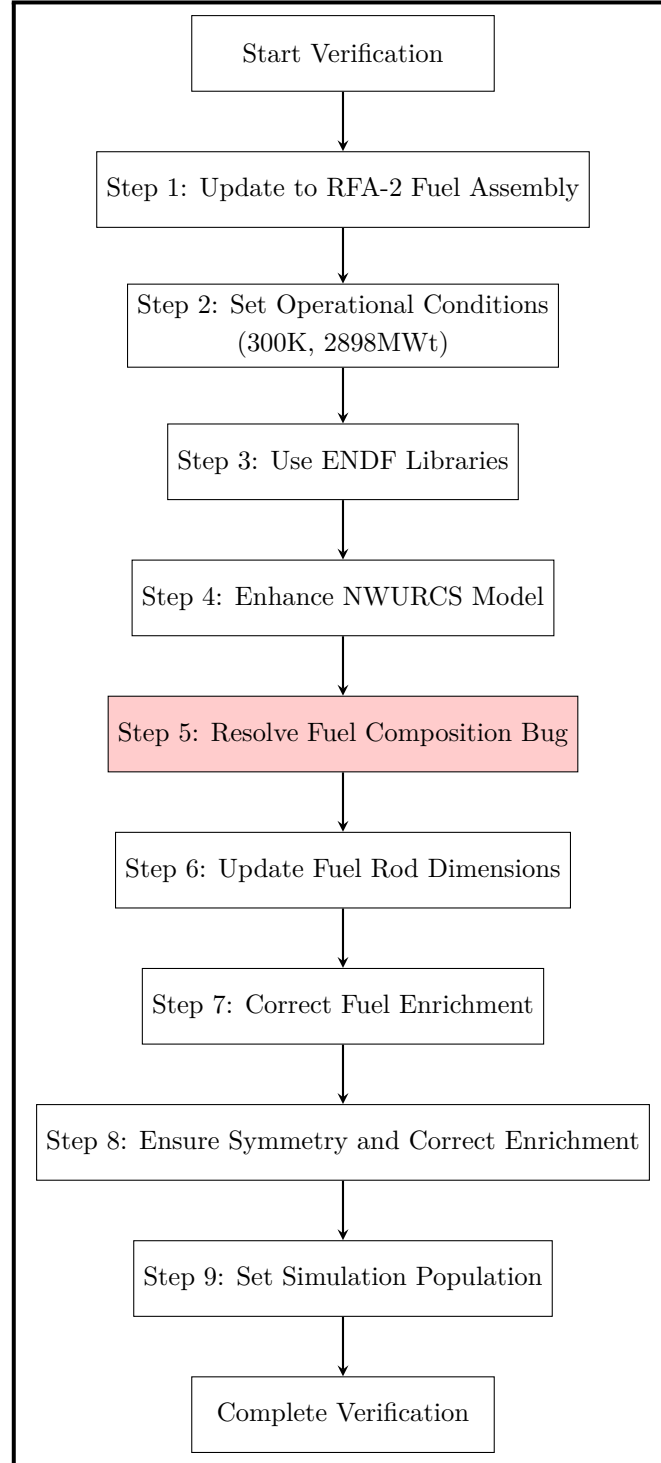


Figure 4.7: Verification process flowchart for neutronic model

Table 4.5 presents the effect of each step on the model's k_{∞} and shows the differences in k_{∞} between the two models with each modification. The k_{∞} pcm value is determined to

be 54 by the conclusion of step 9, indicating that the models demonstrate an adequate level of accuracy and verification.

	Manual model	NWURCS model	kinf difference (pcm)
Step 1	$1.3151 \pm 2.90\text{E-}05$	$1.3176 \pm 7.90\text{E-}05$	143 ± 8.4155
Step 2	$1.3205 \pm 2.90\text{E-}05$	$1.3180 \pm 7.10\text{E-}0.5$	146 ± 7.6694
Step 3	$1.3199 \pm 2.90\text{E-}05$	$1.3180 \pm 7.10\text{E-}05$	109 ± 7.6694
Step 4	$1.3199 \pm 2.90\text{E-}05$	$1.3244 \pm 7.50\text{E-}05$	260 ± 8.0411
Step 5	$1.3199 \pm 2.90\text{E-}05$	$0.4128 \pm 1.40\text{E-}04$	166457 ± 3.2202
Step 6	$1.3613 \pm 5.00\text{E-}05$	$1.3244 \pm 7.30\text{E-}05$	2043 ± 8.8482
Step 7	$1.5742 \pm 2.10\text{E-}05$	$1.3244 \pm 7.30\text{E-}05$	11981 ± 7.5961
Step 8	$1.3254 \pm 2.60\text{E-}05$	$1.3244 \pm 7.30\text{E-}05$	56 ± 7.7492
Step 9	$1.3255 \pm 7.40\text{E-}05$	$1.32456 \pm 7.50\text{E-}05$	54 ± 10.5361

Table 4.5: Comparison of values of infinite multiplication factor for different steps

4.7 Determining average and hottest fuel assembly power

This section outlines the computational methods for determining the average and the hottest fuel assembly powers, along with the verification and validation process implemented.

4.7.1 Average fuel assembly

After verifying the manual full-core model against the NWURCS model, with minor differences noted in k_{eff} and associated errors, the research proceeded with the NWURCS model. An example from the Serpent Wiki regarding pin power distribution was utilised, which included a Serpent mesh-detector code and a corresponding Octave script for visualisation. The mesh-power command was modified to account for the full-core, enabling the representation of fuel assembly power distribution through a MATLAB script adapted from the original Octave script.

The MATLAB code was modified to compute the total core power through the summation of all fuel assembly powers. It was adapted to detect the maximum fuel assembly power within the core and provide the coordinates of the corresponding fuel assembly's location in the reactor core. The average core power, obtained by dividing the total core power by the number of assemblies, was calculated as 18,721 kW. The peaking factor was determined based on the ratio of the maximum fuel assembly power to the average core power. Results of the average fuel assembly power value are presented in Section 5.1

4.7.2 Hottest fuel assembly

The MATLAB code was developed to calculate F_Q for determining the power value of the hottest fuel assembly. The calculated F_Q was 1.93, corresponding to a hottest fuel assembly power of 36,144 kW. However, the value of F_Q was significantly high, as noted in Section 5.1, raising concerns about potential coolant boiling. The initially calculated value of F_Q was not adopted; instead, the recorded value of $F_{N\Delta H}$ from the SAR was used. The SAR provided a reactor condition closely matching the modeled reactor, as illustrated in Figure 4.8. From this condition, the measured $F_{N\Delta H}$ value of 1.21 in the core power map was selected to represent the hottest fuel assembly, rather than the calculated $F_{N\Delta H}$ value shown at the bottom right of the figure. The measured core power map $F_{N\Delta H}$ is based on validated in-core instrumentation and operational data, minimising modelling errors when applied in coupled simulations. $F_{N\Delta H}$ was selected for calculating the power value of the hottest fuel assembly instead of F_Q , due to its ability to reduce DNB during incidents, which is essential for reactor design and safety operations [108]. The hottest fuel assembly power using $F_{N\Delta H}$ was determined as 2,652.24 kW 5.1.

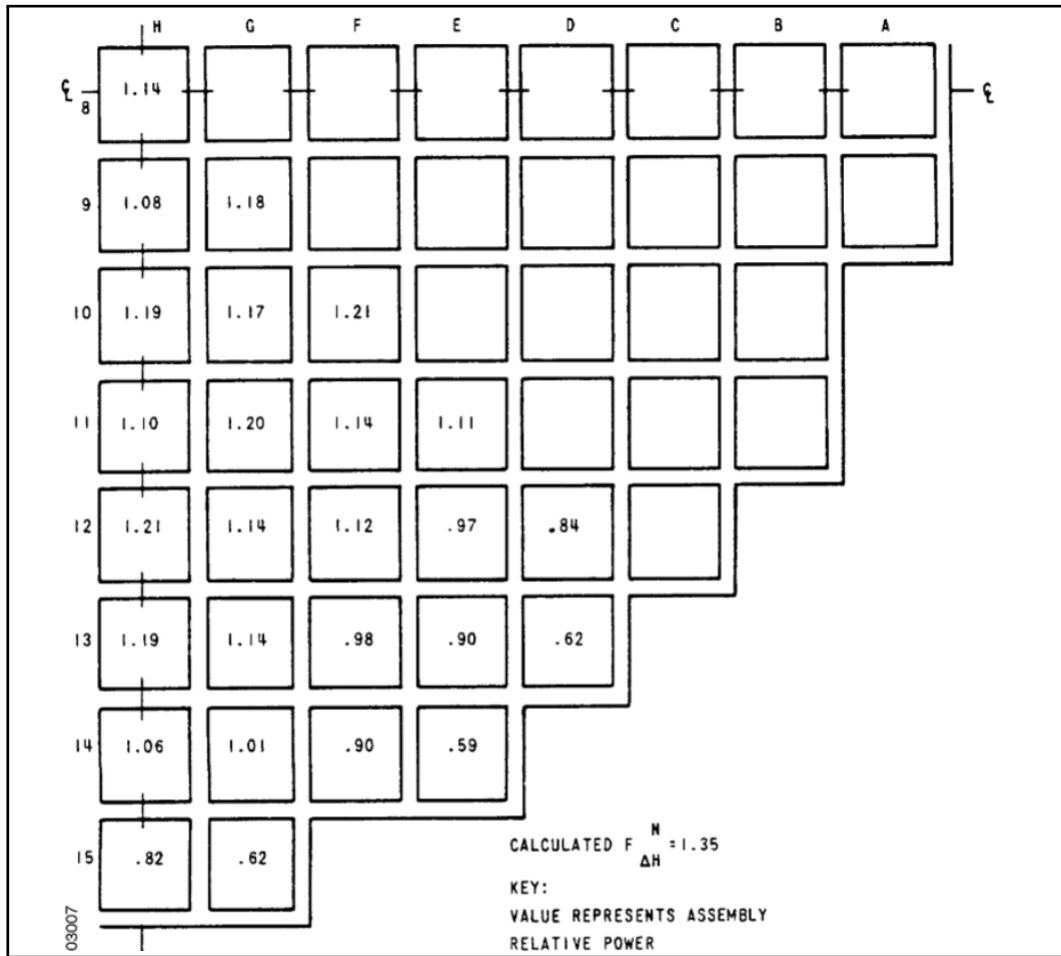


Figure 4.8: Normalised power density distribution near beginning of life, unrodded core, hot full power, no xenon [1]

4.7.3 Verification and validation

According to the definition of Shannon entropy is essential for ensuring the statistical reliability of a simulation. If a volume-distributed fission neutron source has not converged properly, it may lead to skewed power distributions, thereby affecting the power values for both the average fuel assembly and the hottest fuel assembly. Extracting power values before the source reaches equilibrium could result in TH errors in the reactor, which must be accounted for in the safety analysis.

The power values were determined by plotting the Shannon entropy graph, which confirmed that the entropy had stabilised. This stabilisation indicates that the Monte Carlo simulation reached a steady-state neutron population. This further validated that these power values are representative of actual reactor conditions. Refer to the Figure 4.9.

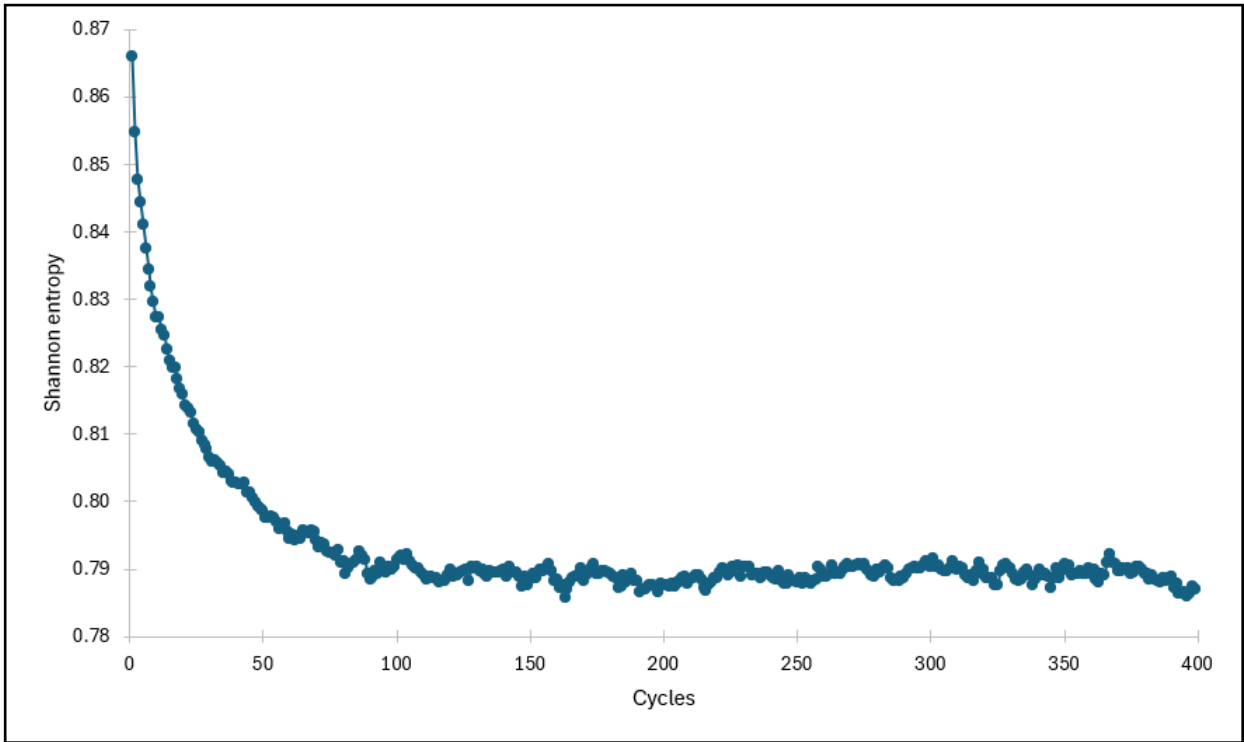


Figure 4.9: Full-core Shannon entropy

Figure 4.9 illustrates the Shannon entropy as a function of the number of cycles for a simulation with set pop 100000 300 100. The entropy decreases rapidly during the initial cycles, reflecting the system's progression toward equilibrium. After approximately 120 cycles, the curve flattens and fluctuates around a stable value, indicating that the neutron source distribution has largely converged. This behaviour confirms that the system transitions from an initial transient phase to a steady state suitable for tallying.

4.8 Coupling methodology

This section outlines the coupling methodology employed for the average and hottest fuel assembly models, as well as the verification and validation procedures implemented.

4.8.1 Coupling approach detailed process

To initiate the coupling process, boundary conditions were established to create a NWURCS Serpent input file specific to the fuel assembly, instead of the entire core. This method was necessary to focus on the peak temperature region of the fuel assembly. A 2.6% enrichment was selected for the fuel assembly simulations to represent mid-life assembly behaviour. This value lies between the enrichment of fresh fuel (3.1%), which has not undergone significant burnup, and that of depleted fuel (2.1%), nearing end-of-life conditions, thereby providing a representative intermediate state for analysis. No soluble boron was used in this study, and no burnable absorbers were included in the model. The input file was manually constructed to correspond with the material compositions, densities, and structure of the NWURCS RFA-2 fuel assembly.

The following steps represent the procedural outline:

1. **Configure Flownex model** Set up the Flownex model, specifying all required parameters and material compositions.
2. **Initialise environment** Using MobaXterm to set up and execute Serpent calculations on the HPC.
3. **Create input files** Construct a manual Serpent input file for the hottest fuel assembly by employing the power data for the hottest fuel assembly calculated using the $F_{N\Delta H}$ value found in Figure 4.8 of the SAR.
4. **Set initial conditions** In the initial iteration, constant temperatures and densities were assumed. The fuel temperature was set at 901 K, the cladding temperature at 629 K, and the water temperature at 583 K [3]. Develop a Cool.ifc input file, referenced within the manual Serpent fuel assembly input file, to specify the coolant densities and temperatures for each individual pin in the fuel assembly.
5. **Define fuel temperatures** Generate a fuel.ifc input file and reference it within the manual Serpent Fuel Assembly input file to define the homogenised material temperatures inside the fuel pins.
6. **Execute Serpent calculations** Run the Serpent input to generate power output files. Verify the distribution of power across each pin to ensure alignment with the calculated total power for the hottest fuel assembly.
7. **Implementation of relaxation factor** A relaxation factor of 0.5 is applied to power, fuel, and coolant from the second iteration.

8. **Input power distribution** Transfer relaxed power distribution data from the detector file into the Flownex input.
9. **Run steady-state analysis** Execute Flownex to produce output files detailing coolant densities, temperatures, and fuel temperatures for the fuel assembly.
10. **Iterative convergence** Feed densities and temperatures from Flownex into Serpent cool.ifc and fuel.ifc files. Repeat iterations until convergence is achieved.

4.8.2 Average fuel assembly power

N calculations yield the spatial distribution of power generated within the reactor core; however, they do not account for thermal feedback effects arising from temperature variations of the coolant and fuel, as they operate under a steady-state assumption. Therefore, coupling N with TH can provide a more accurate depiction of power distribution across all assemblies in the full-core. To evaluate these effects, the average fuel assembly power model will be coupled to examine how varying operational conditions impact power distribution.

To couple a fuel assembly model, a manual input file was created instead of using the NWURCS input. The files cool.ifc and fuel.ifc were generated, with coolant and fuel temperatures set to be homogeneous. Homogeneous coolant and fuel temperatures, when coupling models, simplify calculations, ensure consistent boundary conditions, reduce computational errors, assist in iterative processes, and allow focus on critical parameters, ultimately enhancing reactor analysis and design [109].

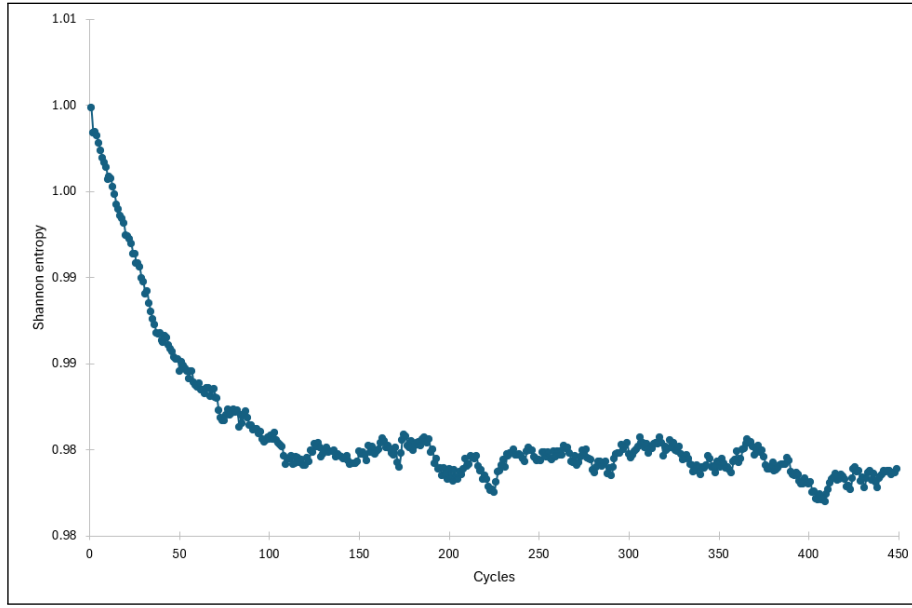
4.8.3 Hottest fuel assembly power

The fuel assembly model was coupled using a consistent manual input file. Boundary conditions in Flownex were adjusted to reflect the new power value calculated in 4.7.2, and a new script was developed to generate updated Flownex views. This was necessary, as the prior Flownex calculations were based solely on the average power model.

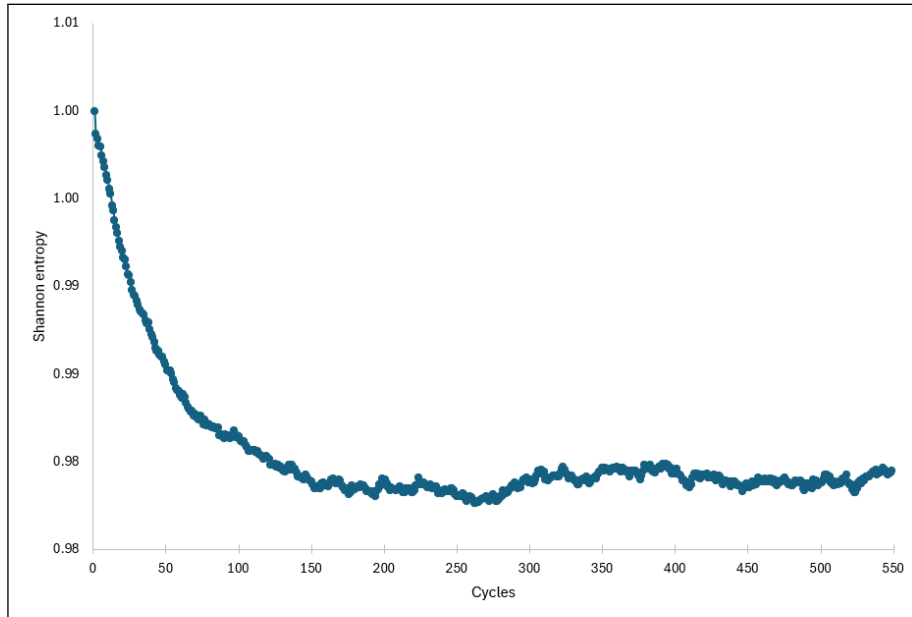
4.8.4 Verification and validation

Figure 4.10 compares Shannon entropies for two different set population commands. Instability in Shannon entropy can result in inaccurate power distributions, influencing fuel temperatures, moderator density, coolant temperature distributions, and potentially causing non-physical reactivity feedback effects. Before coupling, the simulation population settings for the stand-alone fuel assembly model were established using the Serpent command 'set pop 100000 300 150'. This specifies 100,000 neutron histories per cycle, a total of 300 active cycles, and 150 inactive (discarded) cycles to allow the fission source to

converge to the fundamental mode before tallies are collected. This command was subsequently applied during the coupled model run, as illustrated in Figure 4.10a. While this application produced stable entropy, the statistical error was recorded at 17 pcm, surpassing the target threshold of less than 10 pcm. Following this, a modification to the set pop command was implemented, changing it to 'set pop 400000 300 250' where there are 400,000 neutron histories per cycle, a total number of 300 active cycles and 250 inactive cycles, as shown in Figure 4.10b, which resulted in a statistical error of 8.7 pcm, achieving the target threshold. Figure 4.10b demonstrated greater stability compared to Figure 4.10a.



(a) Fuel assembly coupled Shannon entropy (set pop 100000 300 150)



(b) Fuel assembly coupled Shannon entropy (set pop 400000 300 250)

Figure 4.10: Comparison fuel assembly Shannon entropy

4.9 Determining convergence

Convergence was assessed using criteria defined in the input file f005.i of the NWURCS model, specifically for words 211 to 220. These words correspond to various output fields: Field 1 is k_{eff} , Fields 2 to 6 are fuel temperatures at different radial positions, Field 7 is coolant temperature, and Field 8 is power. Each field includes 10 axial levels, while the fuel temperature fields (Fields 2 to 6) also include 5 radial positions: Field 2 at 0 cm, Field 3 at 0.0745 cm, Field 4 at 0.2234 cm, Field 5 at 0.3723 cm, and Field 6 at 0.4096 cm. The convergence thresholds were set to 0.050 % for k_{eff} , 0.3 % for power, 0.6 % for coolant temperature, and 0.3 % for fuel temperature. Figure 4.11 shows an excerpt from the f005.i file that defines the field convergence criteria used in this study.

1	20.0	31.0	1.0	0.00	19.800	80.200	1.5	900000.0	100.0	1000.0
2	0.0000	150.0000	5.0000	300.0000	1.0	32.0	100000.0	200.0	600.0	1.0
3	2.0	213.0	39.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	2.0	6.25000E-07	2.00000E+01	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
5	2.0	1.0	0.0	0.0	0.0	0.00000E+00	2.0	2.0	2.0	11110000.0
6	300.00	300.00	300.00	300.00	300.00	300.00	300.00	300.00	300.00	300.00
7	2000.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	364.99800	5.000E-05	10.0	1.0	100000.0	300.0	100.0	2000.0	2000.0	2000.0
9	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
10	2.0	3.0	2.0	0.0	0.0	0.0	0.0	0.0	1232.0	1.00000E-03
11	1.00	4000.0	4.760E+06	2.40000E+05	300.00	1.00	1.0	0.20000	1.00000	0.07220
12	0.000E+00	1.500E-06	0.0	90.0	1.00000E+00	9.70000E-01	9.70000E-01	9.70000E-01	9.70000E-01	9.70000E-01
13	9.70000E-01	9.00000E-01	9.00000E-01	9.00000E-01	9.00000E-01	9.00000E-01	9.00000E-01	9.00000E-01	1.00000E+04	4.00000E+00
14	1.00000E-01	1.00000E-01	1.00000E-01	1.00000E-01	1.00000E-01	1.00000E-01	1.00000E-01	1.00000E-01	0.00000E+00	0.00000E+00
15	5.0	8.0	8.0	8.0	0.0	0.0	0.0	0.0	0.0	0.0
16	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
17	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
18	6.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
19	10.0	2000.0	1.00000E-05	1.00000E-05	6.0	0.0	0.0	0.0	0.0	0.0
20	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
21	0.0	0.0	2.0	100.0	1.0	32.0	0.0	0.0	99.0	99.0
22	0.050	0.30	0.30	0.30	0.30	0.30	0.60000	0.30	0.00	0.00
23	2.0	0.5	2.0	0.5	0.0	0.0	0.0	0.0	0.0	0.0
24	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
25	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
26	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
27	WORD 211	WORD 213	WORD 215	WORD 217	WORD 219					
28	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
29	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
30	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Figure 4.11: NWURCS manual for convergence

The convergence criteria for power maximum epsilon relative to iterations and centerline fuel temperature maximum epsilon with respect to iterations were established at 2 %. This threshold was determined based on the limitations on the potential for further reduction.

Achievement of convergence is defined by meeting the criteria for all specified fields during the iterative process.

4.10 Conclusion

This chapter presents the rationale for code selection and the advantages of coupling Serpent and Flownex for analysing reactor behaviour. The SAR was utilised to adjust the models in accordance with the latest fuel assembly-RFA-2 configuration. Calculations for Zirlo compositions were conducted due to the transition from Zircalloy to Zirlo cladding in the updated assemblies. A precise representation of the model is critical for generating accurate coupling results, which is instrumental in verifying compliance with established

safety standards. Furthermore, the chapter discusses the necessary procedures for developing both the N and TH models for coupling, followed by a verification and validation process to ensure the coupling's accuracy and reliability.

The subsequent chapter will outline the results obtained from the methodology described in this chapter.

Chapter 5

Results and discussions

This chapter presents the pin-by-pin fuel assembly results for the average fuel assembly and hottest fuel assembly models, along with the overall core results derived from Serpent simulations. The coupling results for the average and hottest fuel assembly models are analysed, focusing on the fields of power, infinite multiplication factor, coolant temperature, and fuel temperature. The objective of this analysis is to evaluate the effectiveness of the coupling and to compare its accuracy to the SAR.

5.1 NWURCS full-core

Following the discussions in Section 4.7.1 and Section 4.7.2, the results generated by the NWURCS Serpent input file and MATLAB code are presented. Refer to Figure 5.1 for the power distribution of the NWURCS full-core model.

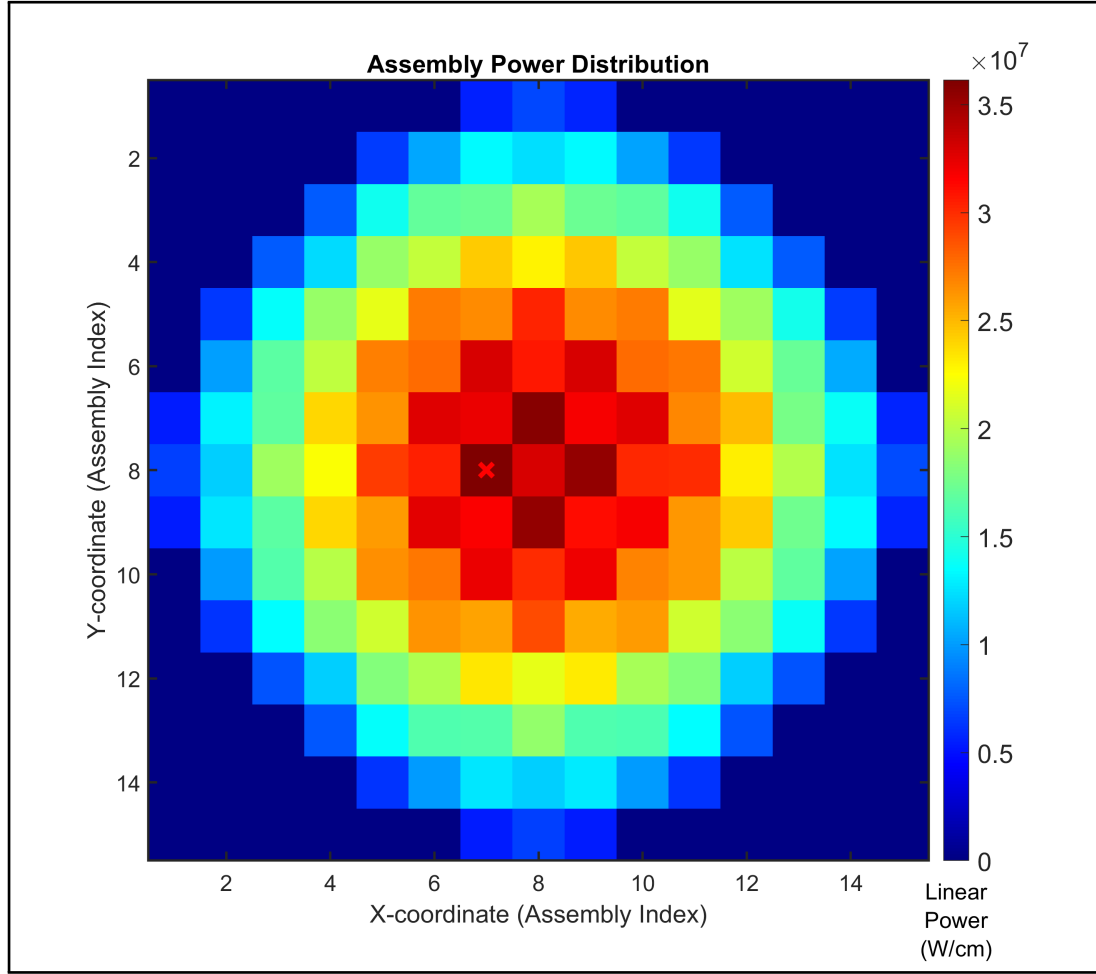


Figure 5.1: NWURCS full-core power distribution

The results obtained are as follows:

Table 5.1: Full-core power distribution results

Parameter	Value
Total core power	2,939,175 kW
Hottest fuel assembly power	36,144 kW
Coordinates of hottest fuel assembly	(X : 7, Y : 8)
Average fuel assembly power	18,721 kW
Fuel assembly F_Q	1.93

The res.m file generated by Serpent recorded the k_{eff} at 1.2656. After accounting for statistical errors, the calculated total core power aligns closely with the operational power set at 2,940,000 kW, showing a discrepancy of only 0.03 %. This confirms the accurate application of the power input. The average fuel assembly power calculated supports the reliability of the MATLAB code utilised, as it corresponds to the total core power divided by the number of assemblies in the core. However, Serpent provided an inaccurate power value for the hottest fuel assembly of 1.9307, which is excessively high. This discrepancy

may result from localised variations in reactor cores, where specific regions exhibit elevated power densities due to factors such as fuel composition, neutron flux, and TH. Despite accurate total power output, these localised power fluctuations—particularly near control rods or in areas with fewer coolant channels—can lead to high peaking factors. Consequently, this contributes to an inaccurate representation of the hottest fuel assembly. Using the $F_{N\Delta H}$ value of 1.21, as noted in Figure 4.8, the determined power value for the hottest fuel assembly that was used for coupling is 22,652.24 kW.

5.2 Average fuel assembly results

Following Section 4.8.2, this section discusses the results obtained from the pin-by-pin coupling of N and TH for the average fuel assembly. The `res.m` file generated by Serpent recorded the k_∞ at 1.2945.

5.2.1 Power results

This subsection addresses the results pertaining to the power of the average fuel assembly model.

5.2.1.1 Power epsilon vs. Iterations

In Iteration 1 of Figure 5.2, the simulation begins with an initial temperature guess, which means that no epsilon value can be calculated yet. The application of an under-relaxation factor of 0.5 in Iteration 2 decreases numerical fluctuations by dampening changes between Iterations. However, due to the value of epsilon being calculated using Equation 3.11, the epsilon value of Iteration 2 is not represented in the plot. Analysis of the graph starting from Iteration 3 reveals an epsilon value of 10.59 %, indicating a significant difference between the first two Iterations. This observation is consistent with the system's adjustment to the coupling effects. A notable decrease occurs in Iteration 4; however, fluctuations persist, indicating ongoing corrections. Between Iterations 5 and 6, a sharp decline is observed, reducing the epsilon value to 1.57 % by Iteration 6. This trend suggests that primary numerical corrections have been implemented, facilitating the system's approach to stability.

Minor fluctuations were observed from Iterations 7 to 10, ranging from 1.74 % to 3.22 %. This behaviour is typical in coupled solutions, as the different domains (N and TH) iteratively adjust to one another. The presence of fluctuations indicates that the system is in the process of refinement, though it has not yet fully converged. A notable spike occurred in Iteration 17, potentially resulting from a numerical feedback effect or an overcorrection in one parameter, thereby influencing the power distribution. The under-relaxation factor of 0.5 mitigates the effect of this spike, preventing more significant oscillations.

Epsilon values remain below 2.28 % from Iterations 18 to 22, indicating system stabilisation. Minor peaks are observed in Iterations 23 and 27. These fluctuations may suggest that localised adjustments are still ongoing, potentially due to delayed numerical feedback between coupled N and TH. Although these peaks are insufficient to indicate divergence, they reveal the presence of residual oscillations. By Iteration 30, the significance of these oscillations decreases, reflecting enhanced stability.

Epsilon values from Iterations 31 to 36 consistently remain below 2 %, indicating stability without significant fluctuations. The median power epsilon across these Iterations is calculated at 1.60 %, suggesting that the power values are closely clustered around the median, further supporting the indication of stable convergence. The standard deviation is 0.08 %, indicating a narrow grouping of fuel temperature values around the median. This suggests stable convergence in the data.

Although Iterations 31 to 36 exhibit convergence, Iteration 34 is selected as the representative converged Iteration for the average assembly, as it yields the lowest epsilon value of 1.58% among this range.

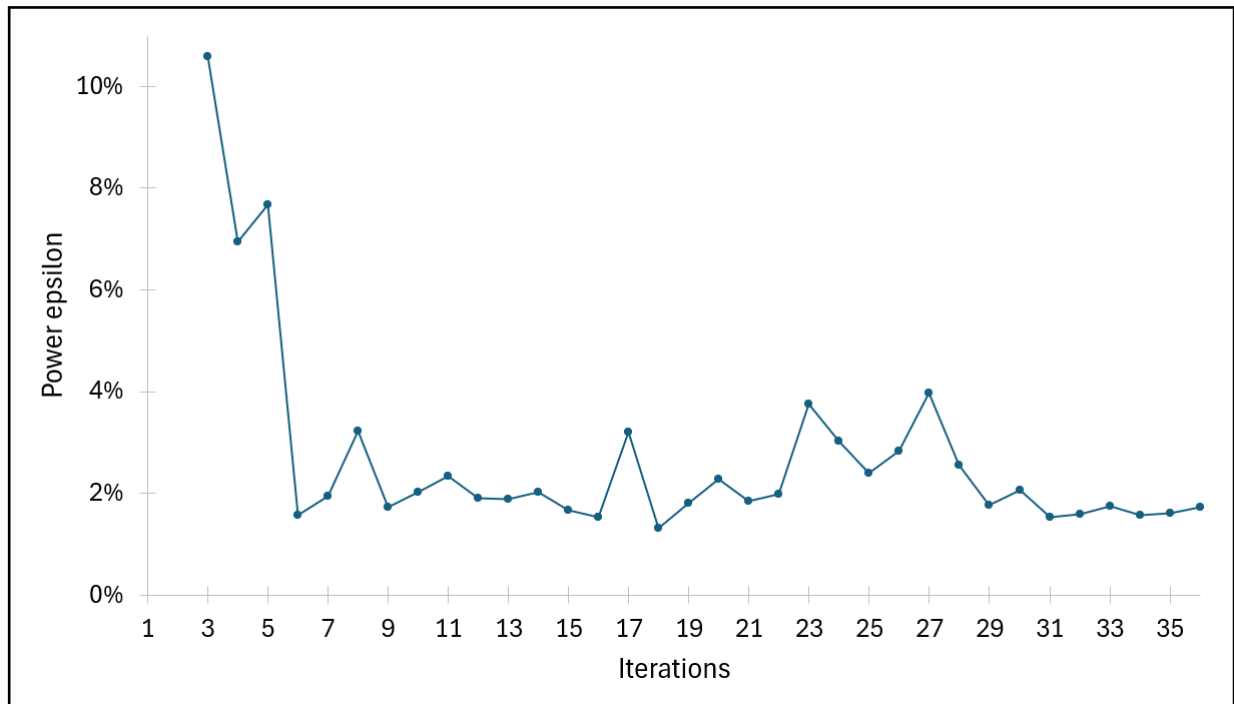


Figure 5.2: Power distribution with Iteration for the average fuel assembly

The pin power distribution of the average assembly is presented in Figure 5.3, with the corresponding numerical values summarized in Table 5.2.

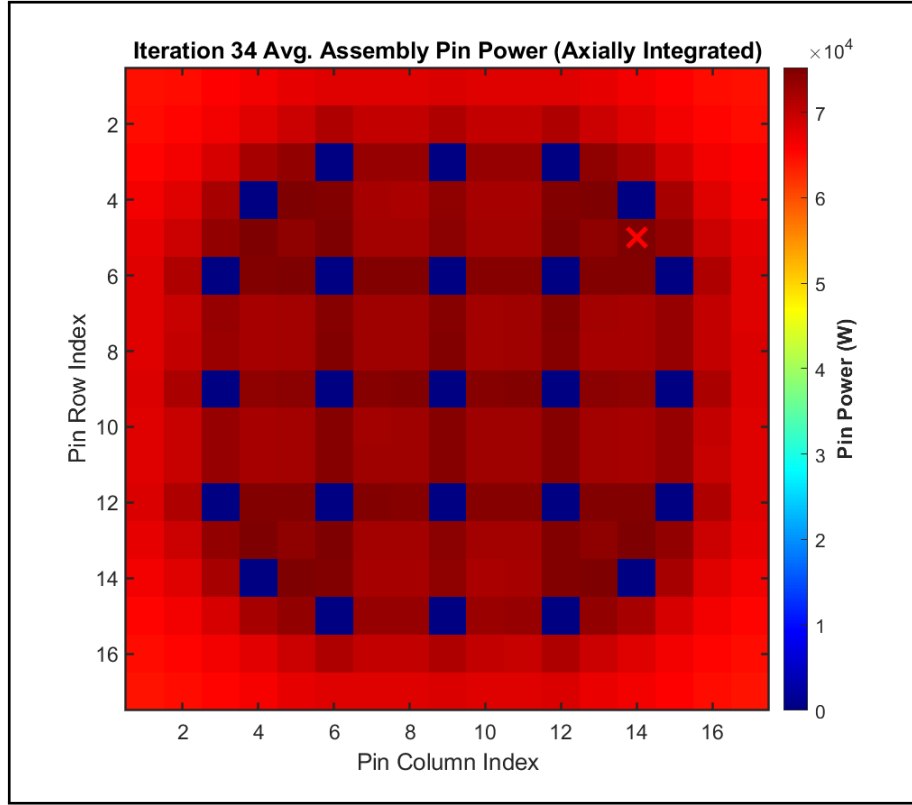


Figure 5.3: Pin power distribution of the average fuel assembly for the converged Iteration (Iteration 34)

Table 5.2: Average assembly pin power distribution results

Parameter	Value
Total assembly power	18,719,551 W
Max pin power (axially integrated)	75,248 W
Average pin power	64,773 W
Assembly pin peaking factor	1.16
Max pin location (Row, Column)	(5, 14)

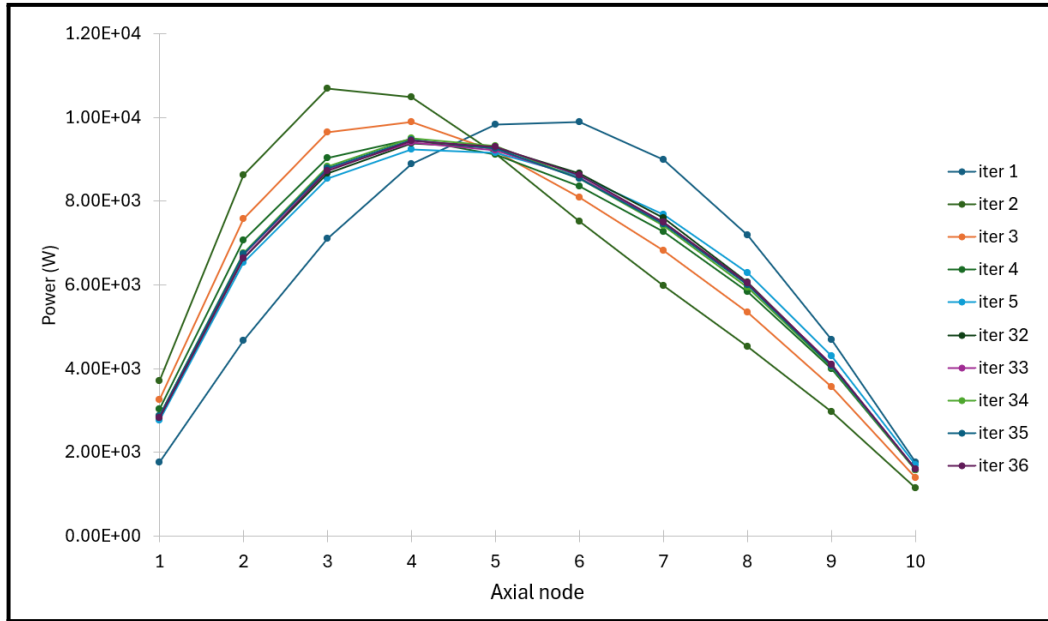
5.2.1.2 Power axial profiles

Analysis of Figure 5.4a shows that excluding relaxation, power profiles exhibit variations across Iterations. This is particularly evident in Iterations 2 and 3, where the profile does not maintain constancy among Iterations. These variations in peak areas are attributed to initial temperature estimates that differ significantly from converged variables, causing discrepancies in power distributions. The system demonstrates sensitivity to temperature changes, leading to feedback effects between neutron flux and coolant temperatures. Serpent calculates power based on these initial temperature estimates, resulting in an unstable axial profile. As Iterations progress, the estimated temperatures begin to converge, although fluctuations remain evident. The substantial changes in temperature estimates

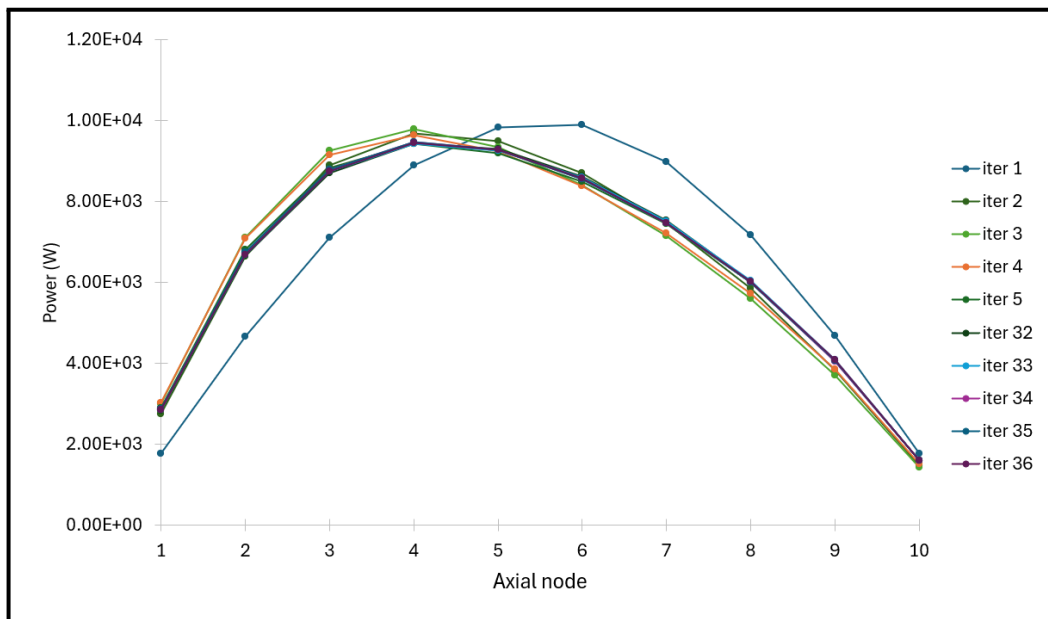
during each Iteration contribute to overshooting and undershooting, which delays convergence. In the final Iterations, the estimated temperatures align more closely with the convergence values, leading to the stabilisation of the axial profiles. However, due to earlier instabilities, minor fluctuations continue to be present for additional Iterations. Consequently, convergence is achieved, though it requires extended computational time.

The power profiles illustrated in Figure 5.4b show increased uniformity across Iterations, indicating the stabilisation of the coupled solution. The relaxation factor limits changes in the estimated temperature per Iteration, thereby minimising abrupt fluctuations in power. While axial power still experiences fluctuations, these deviations are smaller compared to the unrelaxed scenario. By smoothing the transition, the relaxation factor aligns the new temperature estimate closer to the final converged temperature during each Iteration. This method reduces extreme corrections and supports a more rapid stabilisation of the axial power distribution. Convergence to a stable, minimally fluctuating solution between the N and TH solvers improves as the process progresses. In the final Iterations, the estimated temperatures converge with minimal oscillation. Subsequently, the power profile stabilises, as both the N and TH achieve agreement on the steady-state solution. The relaxation factor contributes to enhanced convergence by minimising unnecessary corrections in earlier Iterations.

The simulation encompassed 36 Iterations; however, power axial profiles from only the first five and the final five Iterations are presented for clarity. The initial Iterations reveal rapid fluctuations attributable to feedback adjustments, while the final Iterations indicate a stabilised solution. Intermediate Iterations have been excluded due to their gradual transition, which did not contribute significantly to new insights.



(a) Power axial profile without relaxation



(b) Power axial profile with relaxation

Figure 5.4: Comparison of power axial profiles with and without relaxation

5.2.2 Centerline fuel temperature

This subsection addresses the results pertaining to the centerline fuel temperature of the average fuel assembly model.

5.2.2.1 Centerline fuel temperature vs. Iterations

For the centerline fuel temperature plot, values are advanced by one step; this is due to immediate updates in fuel temperature following power calculations from Serpent. Thus, the plot extends from Iteration 2 to 35, since the power update appears one Iteration later, requiring updated temperature data for recalculation. At Iteration 2, as shown in Figure 5.5, the recorded epsilon value is 8.65 %. This value is anticipated, given that the initial conditions diverge from the true solution. This finding aligns with the system's adaptation to the coupling effects. Between Iterations 2 and 6, a significant decline is noted, decreasing the epsilon value to 0.48 % by Iteration 6. This trend indicates that primary numerical corrections have been applied, contributing to the system's progression toward stability and convergence.

Minor fluctuations were observed in Iterations 7 to 15, ranging from 0.32 % to 0.82 %. This behaviour is typical in coupled solutions, as the different domains (N and TH) iteratively adjust to one another. The presence of fluctuations indicates that the system is in the process of refinement, though it has not yet fully converged. A significant spike was observed in Iteration 16 for the centerline fuel temperature, similar to the patterns seen in power.

Epsilon values remain below 2.28 % from Iterations 17 to 21, indicating system stabilisation. Minor peaks are observed in Iteration 22. These fluctuations may suggest that localised adjustments are still ongoing, potentially due to delayed numerical feedback between coupled N and TH. While these peaks do not indicate divergence, they suggest the existence of residual oscillations. By Iteration 23, the significance of these oscillations diminishes, reflecting increased stability.

Epsilon values from Iterations 23 to 34 remain consistently below 2 %, indicating stability without significant fluctuations. A spike is observed in Iteration 35; however, this value is still below the convergence criterion. Subsequent Iterations would clarify whether the temperature epsilon would remain within the convergence criterion or if additional spikes would occur. The median fuel centreline temperature epsilon across these Iterations is calculated at 0.47 %, consistently below the established convergence criterion of 2 %. The standard deviation measures 0.11 %, suggesting that the fuel temperature values are closely clustered around the median, reinforcing the conclusion of stable convergence.

The temperature field exhibits greater stability compared to the power field, which shows more delayed numerical effects.

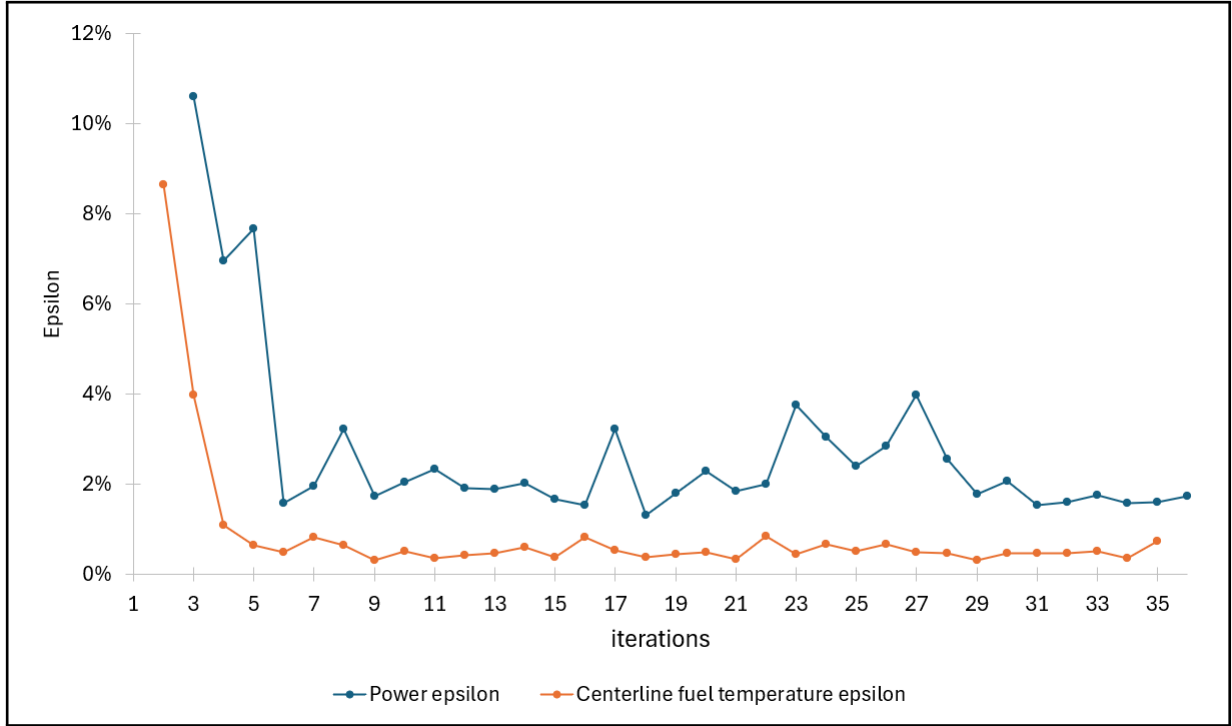


Figure 5.5: Centerline fuel temperature and power variation with Iteration for the average fuel assembly

5.2.2.2 Centerline fuel temperature axial profiles

Figure 5.6 presents the relaxed case of the centerline fuel temperature axial profiles, illustrating variations across Iterations. As Iterations progress, the curves indicate a convergence in fuel temperature distribution, suggesting stabilisation of the temperature distribution within the system.

The fuel temperature profiles of Iterations 1 and 2 exhibit notable differences. This indicates that the initial guessed values of coolant and fuel temperatures were substantially divergent from the final converged solution. Significant adjustments arise from the interactions between the N and TH components of the model.

Iterations 3 to 5 demonstrate a convergence of the profiles, indicating increased similarity while remaining distinct. The system is nearing a stable solution, evidenced by a reduction in the magnitude of adjustments applied with each Iteration.

Iterations 32 to 36 demonstrate that the curves overlap with greater significance, suggesting the absence of further significant changes in the temperature profile. This observation indicates numerical stability and convergence, with the coupled N and TH of the model achieving a self-consistent solution. At this stage, the temperature distribution accurately reflects the combined effects of heat generation in the fuel, heat transfer to the coolant, and feedback from the two solvers.

The simulation encompassed 36 Iterations; however, centerline fuel temperature axial profiles from only the first five and the final five Iterations are presented for clarity. The initial Iterations exhibited rapid fluctuations resulting from numerical feedback adjustments, whereas the final Iterations demonstrated a stabilised solution. Intermediate Iterations have been excluded due to their gradual transition, which did not contribute significantly to new insights.

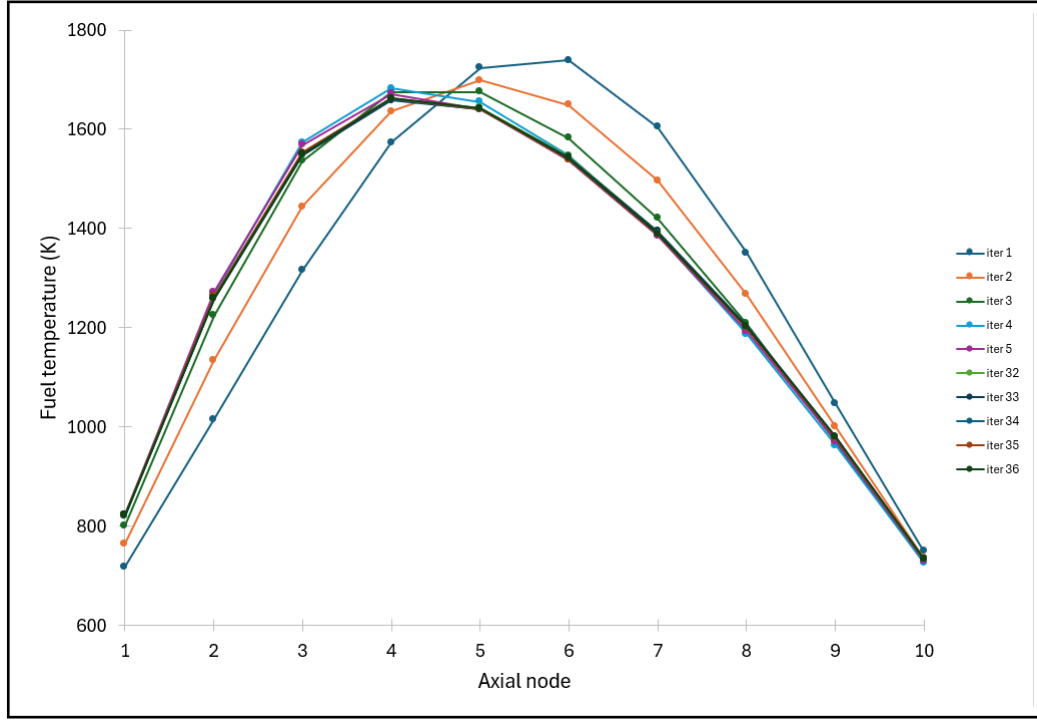


Figure 5.6: Centerline fuel temperature axial profiles for the average assembly

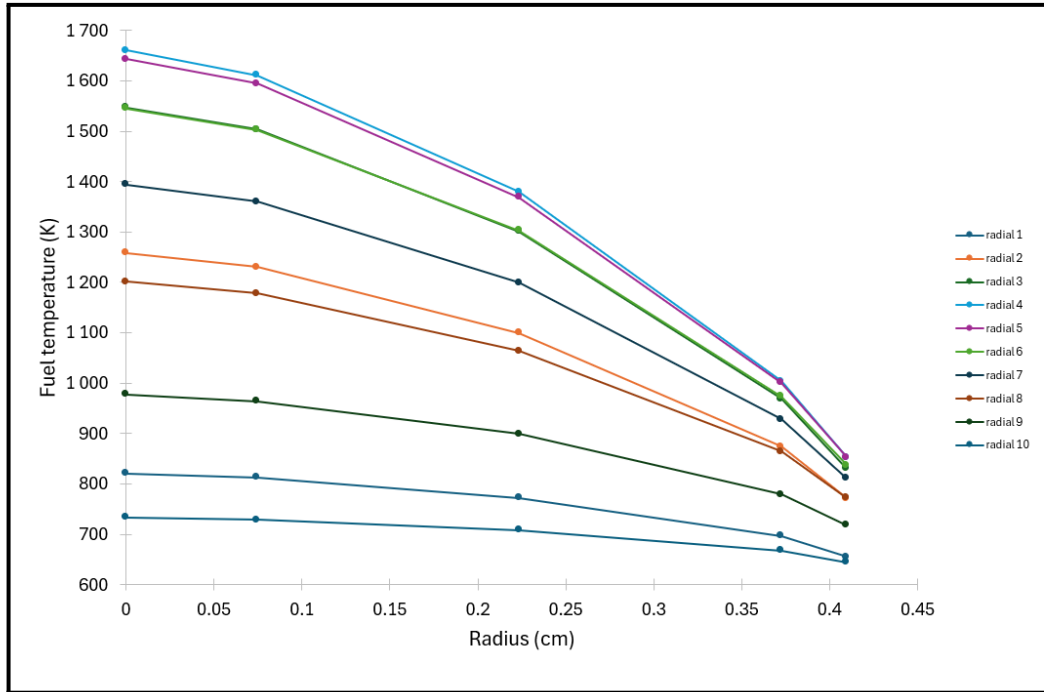
5.2.2.3 Fuel temperature radial profiles

Figure 5.7a illustrates the radial fuel temperature distribution averaged across all pins in Iteration 34 of the average fuel assembly. This Iteration was selected based on the convergence of the centerline fuel temperature epsilon at the same Iteration. The plot demonstrates that the neutron flux reaches its maximum at axial level 4, where the maximum temperature is recorded at 1660.38 K. At this radial position, coolant has absorbed heat from lower levels, leading to decreased cooling efficiency and increased fuel temperatures. This observation indicates a direct correlation between the power peak and localised heat generation.

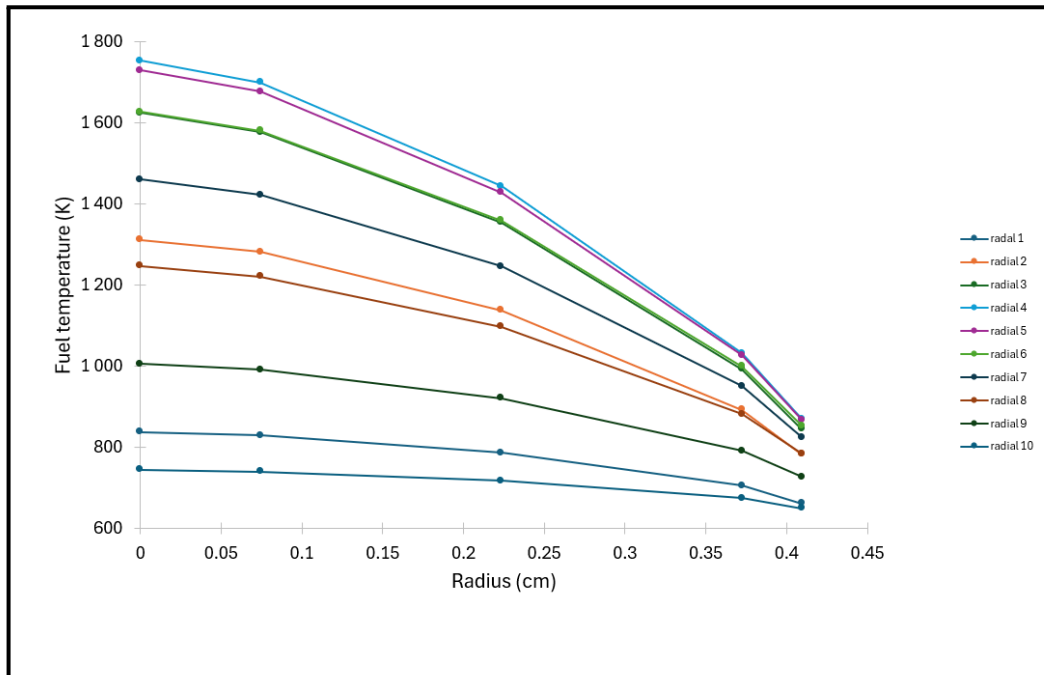
Figure 5.7b is essential for evaluating potential overheating risks within the fuel assembly. It presents the maximum temperature recorded at the hottest pin which is pin 205, which is crucial for assessing safety limits, as excessive temperature may compromise fuel integrity. The data indicate that the peak temperature recorded at radial level 4 is 1753.66 K, resulting in a differential of 93.28 K between the hottest pin and the average pin temperature profile. While the melting temperature establishes a critical upper limit for fuel integrity,

the radial temperature difference serves as a key indicator of thermal distribution within the reactor core. A significant radial temperature difference increases the likelihood that the hottest pin may approach the melting temperature, potentially leading to fuel failure. Therefore, minimising the radial temperature difference is essential for ensuring safe and efficient reactor operation.

Both profiles peak at the same radial level, with a reasonable difference between the two temperatures. This alignment demonstrates an effective coupling of TH and N behaviours, influenced by Doppler and moderator feedback mechanisms, which contribute to power stabilisation. The findings support the conclusion that the observed coupling accurately reflects the operational behaviour of the reactor.



(a) Iteration 34 average pin fuel temperature radial profiles



(b) Highest pin fuel temperature radial profile

Figure 5.7: Comparison of fuel radial profiles in the average fuel assembly

5.2.3 Coolant temperature axial profiles

This subsection presents the results related to the coolant temperature of the average fuel assembly model.

Iterations 1 and 2 of Figure 5.8 show differences in the coolant temperature profiles, indicating that the system has not yet achieved convergence. These variations are due to adjustments made to the initial guess values. The existence of differences between Iterations suggests that the TH solver is adjusting the temperatures based on feedback from both N and TH components of the system.

As Iterations advance from 3 to 5, the curves representing the coolant temperature profile exhibit increased proximity. This trend indicates that the solution approaches convergence, reflecting numerical stabilisation as initial estimates are refined during the iterative coupling process. At this point, a balance begins to form within the system concerning power distribution, coolant flow, and heat transfer.

From Iteration 32, the system attains a converged steady-state solution where the feedback between N and TH is consistent, indicating that the iterative process has stabilised.

The average coolant temperature at the top of the core in axial level 10 of Figure 5.8 is recorded at 590.47 K, based on the Cool.ifc file for the average fuel assembly. This temperature is lower than the value of 600.87 K at the same location, as indicated in Table 4.4-3 represented in Figure C.6, of the SAR [1]. This difference indicates a temperature rise deviation of 26.68 % in the average fuel assembly compared to the rise specified in SAR. The Flownex output node (combining all of the fuel pin channels) records a resultant coolant temperature of 591.47 K, corresponding to a deviation of 24.11 % from the rise indicated in SAR, which is slightly lower. The observed differences between the Flownex output and SAR, in addition to the variations between the Cool.ifc temperatures and the Flownex outputs may be attributed to the surface roughness of Zircaloy-4, as referenced in [107] given the lack of surface roughness data in SAR. The study employs the RFA-2 fuel assembly but lacks critical TH design parameter information in the SAR, including pressure drop details. Insufficient data may contribute to inaccuracies in the results. Moreover, discrepancies could arise from the various tables in SAR related to TH parameters that are not included in the RFA-2 fuel assembly tables, leading to uncertainty regarding the appropriate table for validation.

The simulation encompassed 36 Iterations; however, coolant temperature axial profiles from only the first five and the final five Iterations are presented for clarity. The initial Iterations reveal rapid fluctuations attributable to feedback adjustments, while the final Iterations indicate a stabilised solution. Intermediate Iterations have been excluded due to their gradual transition, which did not contribute significantly to new insights.

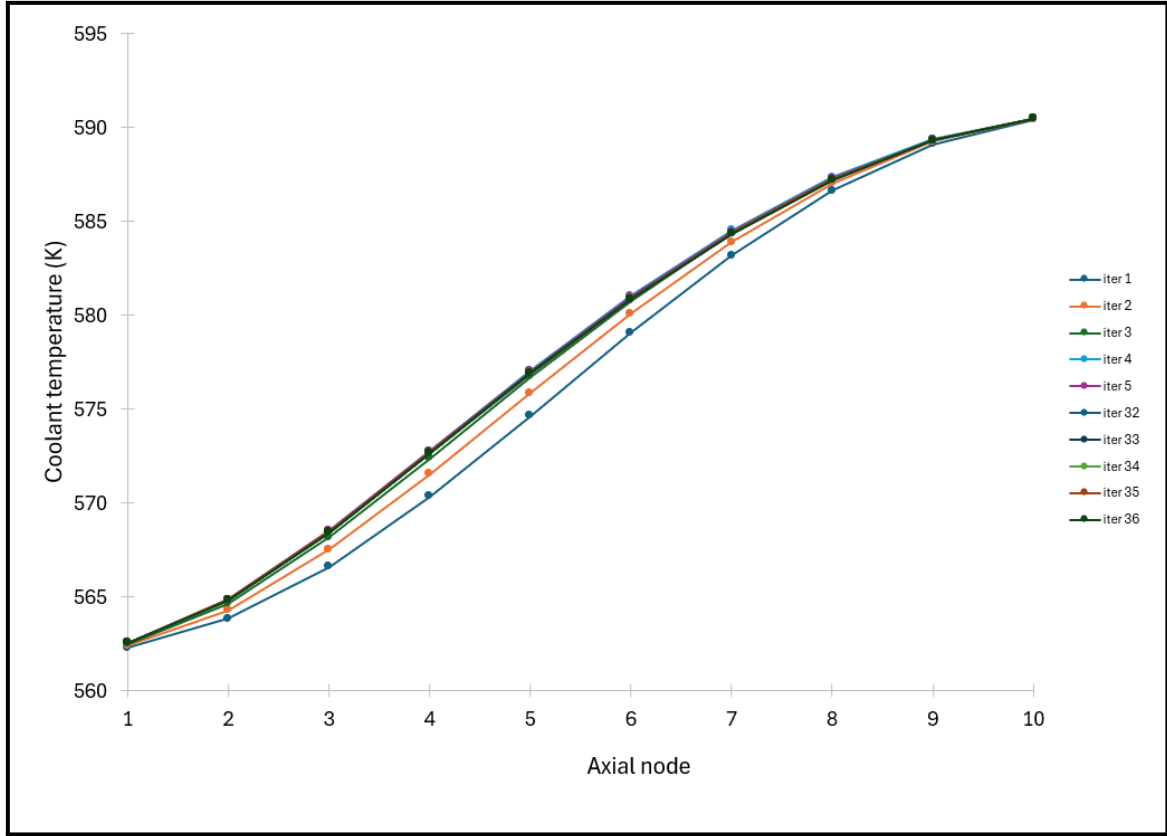


Figure 5.8: Coolant temperature axial profiles

5.2.4 Infinite multiplication factor

This subsection addresses the results pertaining to the infinite multiplication factor of the average fuel assembly model.

5.2.4.1 Infinite multiplication factor vs. Iterations

The first Iteration of Figure 5.9 begins with a high k_{∞} value of 1.298, which subsequently decreases sharply during the initial Iterations. This decline is accounted for by the initial discrepancy between N power and coolant conditions. Initially, k_{∞} remains elevated due to the system's assumption of a preliminary power estimate that does not align with the thermal state. As the coolant temperature increases, the reduction in neutron moderation results in a decrease in k_{∞} , clarifying the observed rapid decline. By Iteration 5, the k_{∞} stabilises at 1.2945, and this marks the transition to numerical stability.

Between Iterations 6 and 15, k_{∞} values display fluctuations in the range band of 30 pcm. These variations are attributed to stochastic Monte Carlo uncertainties present in the results computed with the Serpent code and numerical coupling effects, where minor updates in coolant properties affect neutron moderation. The small amplitude of these fluctuations indicates a trend towards stabilisation of k_{∞} .

Between Iterations 16 to 36, fluctuations in k_∞ are observed, remaining within a range band of 38 pcm. No significant deviations were observed, indicating that the coupled simulation has likely reached a stable solution. Minor variations in k_∞ were anticipated due to Monte Carlo uncertainties; however, this phase supports the conclusion of system convergence. The final Iterations exhibited no considerable drift, suggesting that additional Iterations would not materially affect the final result.

k_∞ indicates the convergence of the multiplication factor from Iteration 5 to 36, characterised by low-amplitude oscillations within a range band of approximately 40 pcm. This range is in proximity to the standard deviation of 26.1 pcm (3 sigma) obtained from a stand-alone Serpent calculation. Additionally, the epsilon values during these Iterations remain below 0.03 %.

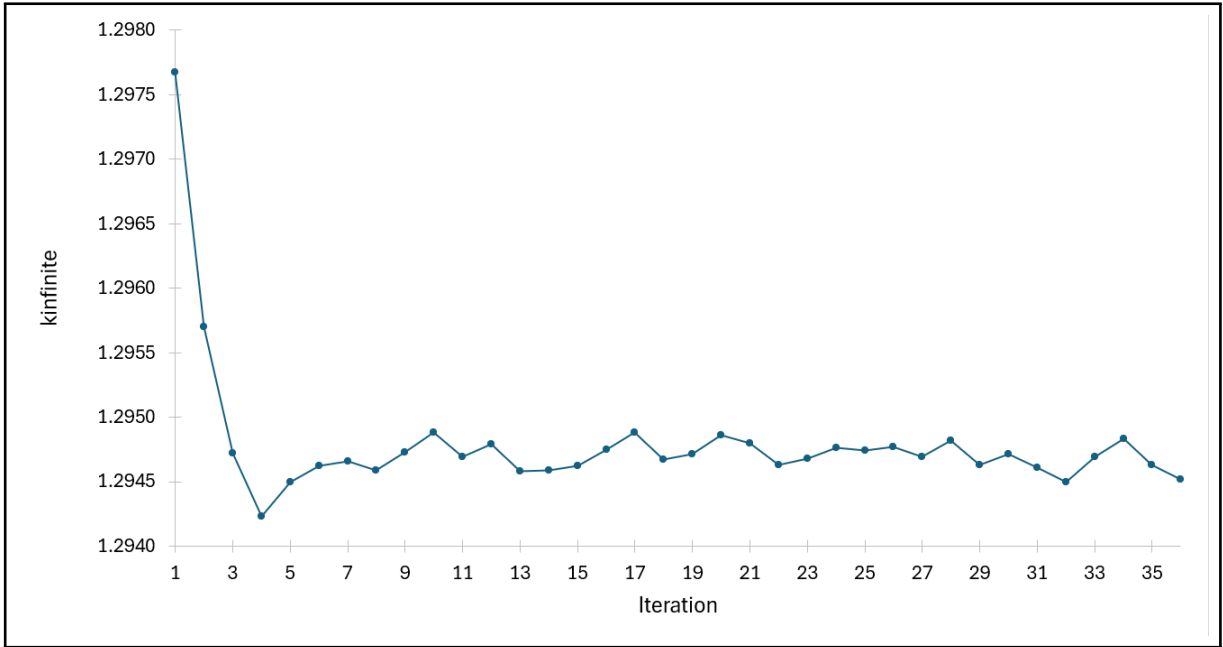


Figure 5.9: Infinite multiplication factor vs. Iterations

5.2.4.2 Variation of infinite multiplication factor and average coolant temperature with Iterations

In Iteration 1, as illustrated in Figure 5.10, the average coolant temperature is determined by averaging all pins in the z-direction, utilising an assumed initial value. This initial value affects density, heat transfer properties, and neutron moderation. The coolant temperature does not accurately reflect the actual power deposition from Serpent, leading to a power distribution that is inconsistent with converged steady-state conditions. This inconsistency results in an initial value of k_∞ at 1.297, paired with a low coolant temperature of 576.62 K. The power distribution prompts an increase in coolant temperature during Iteration 2, as heat transfer mechanisms adjust to the estimated power. This rise in coolant temperature subsequently decreases the density, which impacts neutron moderation and contributes to a reduction in k_∞ . A significant decrease in k_∞ occurs, reaching 1.294 by Iteration 4,

as Serpent adjusts the initially high power predictions. By Iteration 5, both parameters demonstrate stabilised fluctuation, indicating that the feedback mechanism is functioning towards numerical stabilisation.

From Iteration 6 to 15, k_∞ stabilises within a range band of 30 pcm, although minor oscillations are noted. By Iteration 6, the coolant temperature attains 577.82 K and remains stable, as the coupled simulation reveals a consistent correlation among heat deposition from fission, heat transfer, and the mass flow rate of the coolant. Excessive coolant temperature can hinder effective heat removal, posing a risk to DNB. The simulation maintains the coolant at an optimal temperature for efficient heat removal. Flownex updates the coolant temperature based on the latest power distribution from Serpent, while Serpent recalculates k_∞ using these updated coolant temperatures, which influences neutron moderation and power generation. The feedback effect is apparent, as the coolant temperature exhibits limited fluctuations, indicating that the power-temperature relationship is stabilising.

From Iteration 16, both k_∞ and coolant temperature demonstrate minor fluctuations while remaining stable. k_∞ demonstrates a range band of 40 pcm, whereas the coolant temperature shows a range band of 0.07 K from Iterations 16 to 36. These variations suggest that the numerical coupling process has achieved a quasi-static equilibrium, where the output of each solver minimally impacts the other's predictions. The fluctuations in k_∞ may result from statistical uncertainties in Serpent or minor variations in power distribution updates. At Iteration 36, the solution is considered converged, as further Iterations do not produce significant changes.

The plot illustrates the relationship between k_∞ and coolant temperature, emphasising the role of negative reactivity feedback in stabilising the system. This interaction is critical for PWR safety, as it promotes reactor stability and facilitates efficient heat removal.

The plot demonstrates that average coolant temperature convergence begins at Iteration 5, with an epsilon below 0.6 %. The observed range band is 0.09 K, reflecting the amplitude of small oscillations around the convergence point. During these Iterations, the average temperature recorded is 577.77 K, accompanied by a standard deviation of 0.02 K.

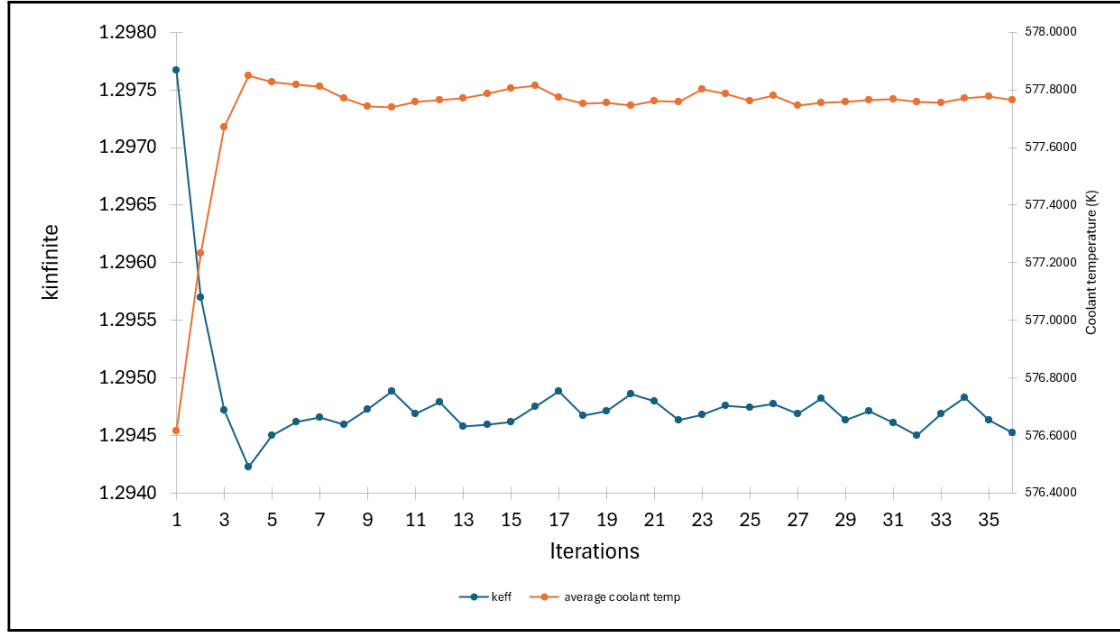


Figure 5.10: Variation of infinite multiplication factor and average coolant temperature with Iterations for the average assembly

5.2.4.3 Variation of infinite multiplication factor and average centerline fuel temperature with Iterations

At Iteration 1 of Figure 5.11, the initial average centerline fuel temperature is computed by averaging all pins in all the z-direction, while the maximum centerline fuel temperature is determined by identifying the peak temperature at any pin location along the z-direction. This estimated value is utilised by the Serpent N solver for the initial power calculation. Serpent computes the k_{∞} based on this initial temperature; however, the power distribution applied in this computation is inaccurate due to overestimation. As a result, the k_{∞} , the average centerline fuel temperature and the maximum centerline fuel temperature, begin at elevated initial values compared to their final converged states. The average centerline fuel temperature at Iteration 1 is 1283.8 K, while the maximum centerline fuel temperature reaches 1657.66 K, and the k_{∞} is recorded at 1.298. Flownex employs this power distribution to recalculate the fuel temperature in Iteration 2. By Iteration 3, the first updated power distribution from Serpent is used by Flownex to recompute the fuel temperature. A slight reduction in k_{∞} , alongside a slight increase in maximum centerline temperature from Iteration 1 to 2. However, both the average and maximum centerline fuel temperatures remain relatively stable from Iteration 2 onward, indicating minimal fluctuations that suggest minor system adjustments as Serpent and Flownex exchange information.

Convergence of centerline fuel temperatures and k_{∞} is observed between Iterations 5 and 36. The average and maximum centerline fuel temperature exhibit minimal fluctuations, measuring 38 pcm for k_{∞} , 1.36 K for average centerline fuel temperature, and 27.99 K for

maximum centerline fuel. This observation indicates numerical convergence. The stable temperature values computed within Flownex imply that significant changes between Iterations have ceased, leading to negligible variations in power and reactivity calculations within Serpent. This stabilisation confirms that the numerical coupling has attained a converged steady-state solution, with epsilon values consistently below the established criterion of 0.3 %. The standard deviation of average centerline fuel temperature across these Iterations is 0.26 K, while the standard deviation of maximum centerline fuel temperature is 6.10 K.

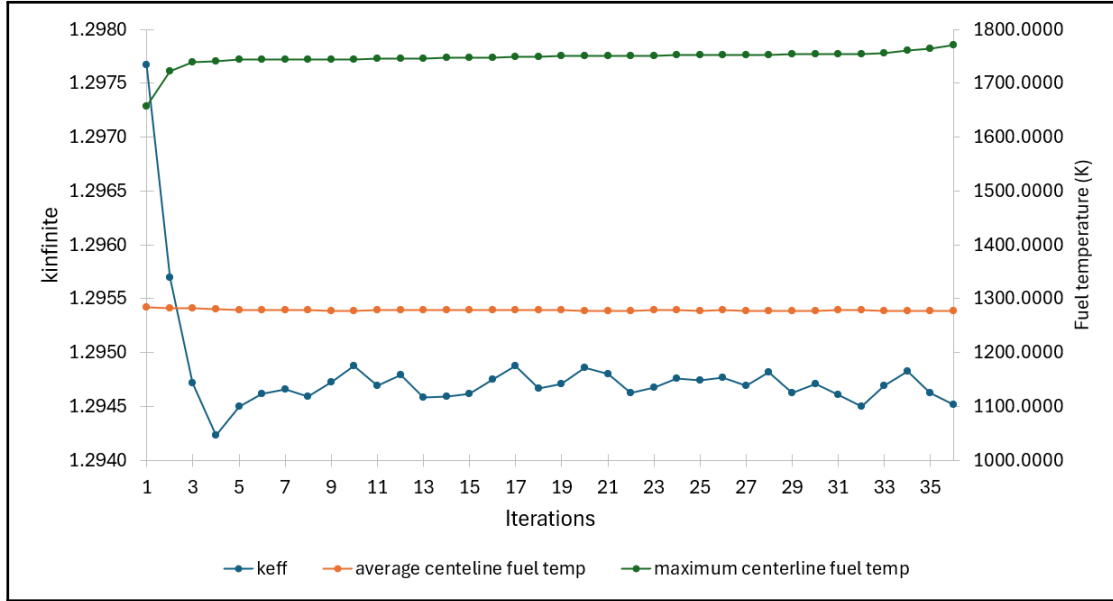


Figure 5.11: Variation of infinite multiplication factor and average centerline fuel temperature with Iterations

5.3 Hottest fuel assembly results

Following Section 4.8.3, this section discusses the results obtained from the pin-by-pin coupling of N and TH for the hottest fuel assembly. The res.m file generated by Serpent recorded the k_{∞} at 1.2890.

5.3.1 Power results

This subsection addresses the results pertaining to the power of the hottest fuel assembly model.

5.3.1.1 Power epsilon vs. Iterations

At Iteration 1 of the hottest fuel assembly shown in Figure 5.12, the simulation initiates with a preliminary temperature estimate. Consequently, the epsilon value cannot be computed, which is also true for the average fuel assembly. Analysis of the graph from Iteration 3 indicates an epsilon value of 11.59 %. At Iteration 4 of the hottest fuel assembly, the epsilon value increases to 15.27 %. This is in contrast to the decrease observed in the average fuel assembly from Iteration 3 to 4. Building on the trend observed in the average fuel assembly, Iterations 5 through 7 of the hottest fuel assembly show a significant decrease, with the epsilon value dropping to 2.05 % by Iteration 7.

Fluctuations between Iterations 8 and 15 of the hottest fuel assembly demonstrated a range band of 0.94 %, which is smaller than the 1.56 % range band observed from Iterations 8 to 15 in the average fuel assembly. The error remained below 2 % during Iterations 9 and 10 of the hottest fuel assembly. However, additional Iterations were conducted to investigate the stability and convergence behaviour of the coupled system. A spike was recorded in Iteration 16 of the hottest fuel assembly, potentially attributed to a numerical feedback effect or an overcorrection in one variable affecting power distribution. Iteration 17 of the average fuel assembly similarly exhibited a spike.

Epsilon values were consistently below 2.61 % during Iterations 17 to 24 of the hottest fuel assembly, suggesting system stabilisation. Minor peaks were observed in Iterations 25, 28, 32, and 35 of the hottest fuel assembly. While these peaks do not suggest divergence, they indicate the presence of residual oscillations.

The calculated power epsilon median for the convergence from Iteration 7 onwards in the hottest fuel assembly is 2.00 %, which slightly exceeds the value for the average fuel assembly at 1.93 %. This finding indicates that most Iterations exhibit stability and potential for convergence, as the median value is marginally above the established convergence criterion of 2 %. The standard deviation across the same Iterations for the hottest fuel assembly is 0.01 %, indicating that power values are closely clustered around the median, further supporting the evidence of stable convergence.

Iteration 34 is identified as the converged Iteration of the hottest assembly, as it yields the minimum epsilon value of 1.24% within the stable range of Iterations 7 to 36, consistent with the converged Iteration of the average assembly.

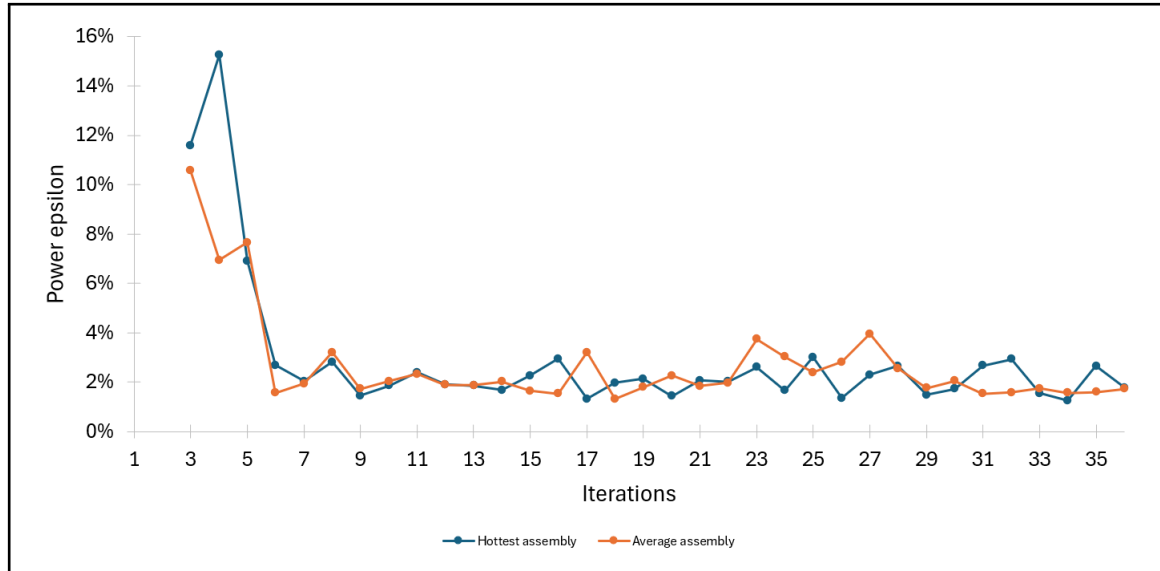


Figure 5.12: Comparison of the power distribution with Iteration for the hottest and average fuel assembly

The pin power distribution of the hottest assembly is presented in Figure 5.13, with the corresponding numerical values summarised in Table 5.3. The table shows that the pin peaking factor, defined relative to the assembly-average power, is 1.16 for both the average and hottest assemblies. For the hottest assembly, the corresponding pin peaking factor relative to the full-core average is 1.40, calculated as the product of the assembly peaking factor (1.21) and the pin peaking factor relative to the assembly (1.16).

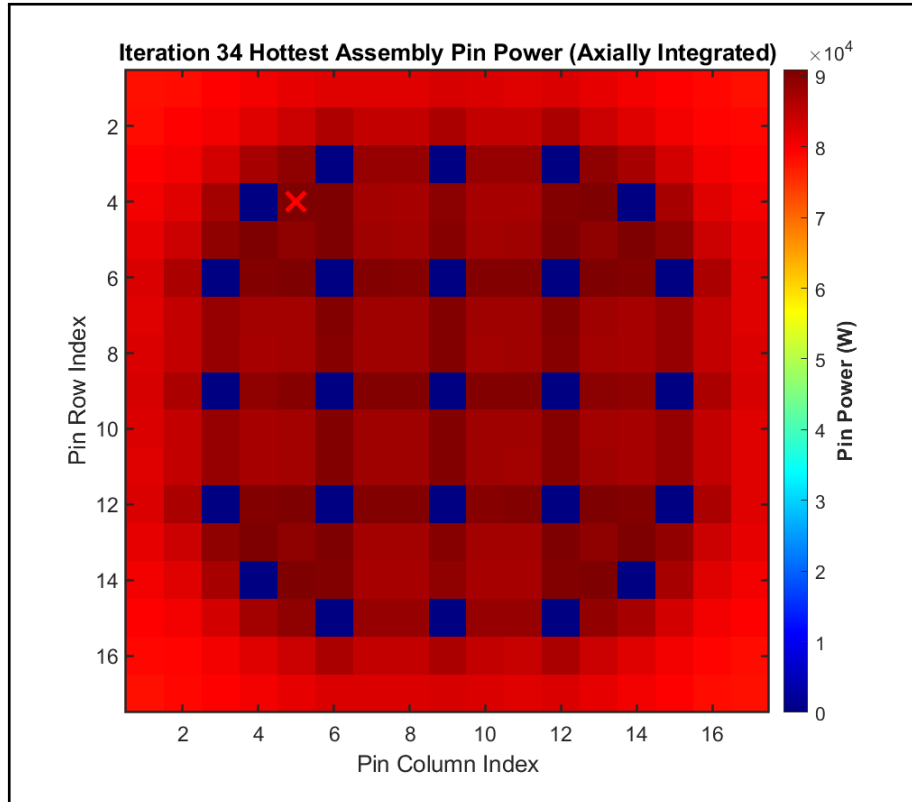


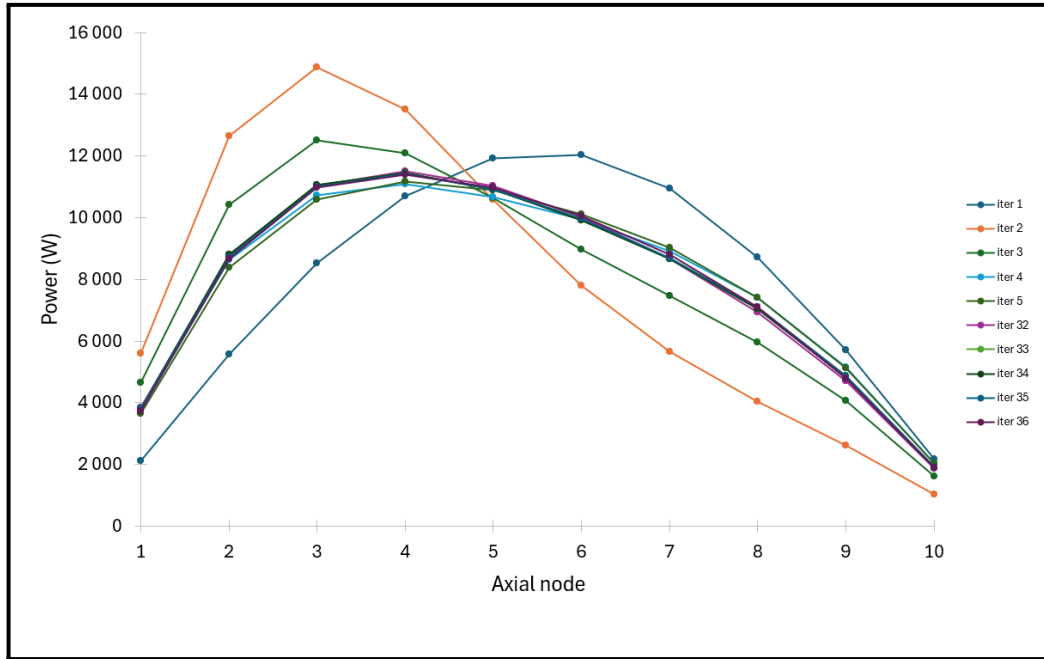
Figure 5.13: Pin power distribution of the hottest fuel assembly for the converged Iteration (Iteration 34)

Table 5.3: Hottest assembly pin power distribution results

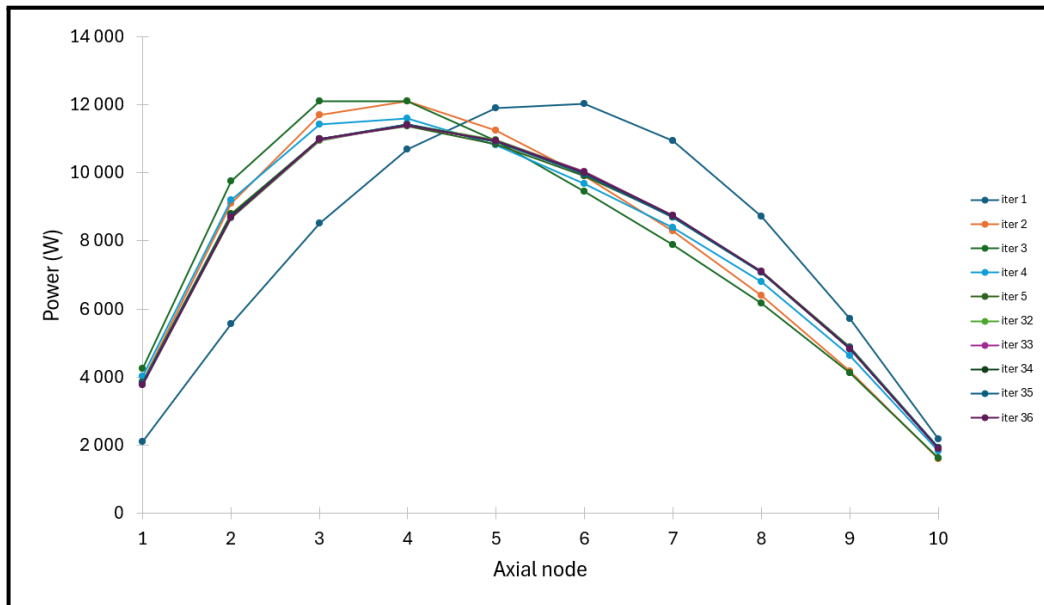
Parameter	Value
Total assembly power	22,651,597 W
Max pin power (axially integrated)	90,933 W
Average pin power	78,379 W
Assembly pin peaking factor	1.16
Max pin location (Row, Column)	(4, 5)

5.3.1.2 Power axial profiles

The axial power profiles of the hottest fuel assembly, excluding and including relaxation, as shown in Figure 5.14, demonstrate a trend comparable to that of the average fuel assembly presented in Figure 5.4. The power values for the hottest fuel assembly are consistently higher than those of the average fuel assembly, with a peak value of 14.89 kW observed in Figure 5.14a, contrasting with the 9.64 kW recorded in Figure 5.4a for the average fuel assembly prior to relaxation. Furthermore, Figure 5.4b indicates a more rapid convergence compared to Figure 5.14b following relaxation.



(a) Power axial profile without relaxation



(b) Power axial profile with relaxation

Figure 5.14: Comparison of power axial profiles with and without relaxation of the hottest fuel assembly

5.3.2 Centerline fuel temperature

This subsection addresses the results pertaining to the centerline fuel temperature of the hottest fuel assembly model.

5.3.2.1 Centerline fuel temperature vs. Iterations

In Iteration 2, the peak centerline fuel temperature for both the hottest fuel assembly and the average fuel assembly, as presented in Figure 5.15 offers an initial estimate for numerical coupling. In Iteration 2, the fuel temperature epsilon for the hottest fuel assembly is recorded at 13.39 %, which is higher than the 8.65 % recorded for the average fuel assembly, attributed to the greater power output of the hottest fuel assembly. The hottest fuel assembly exhibits a similar trend to the average fuel assembly, declining to a low epsilon value of 1.42 % by Iteration 8. From Iteration 16 to 18, an observable spike in epsilon occurs within the hottest fuel assembly. Subsequently, fluctuations are noted from Iteration 18 to 30 in the hottest fuel assembly, maintaining a range band of 3.25 %, in contrast to the narrower range band of 0.53 % seen in the average fuel assembly during the same Iterations. Post Iteration 30, the hottest fuel assembly's fuel temperature appears to stabilise; however, a spike is recorded in Iteration 35. Additional Iterations could have been conducted to assess whether the trend would continue to oscillate or converge, similar to the behaviour of the average fuel assembly. The median centerline fuel temperature for the hottest fuel assembly from Iteration 7 onward is 2.51 %, compared to 0.47 % for the average fuel assembly. The standard deviation of the centerline fuel temperature for the hottest fuel assembly is 2.09 % within the same Iterations, whereas the average fuel assembly exhibits a standard deviation of 1.15 %. The lower standard deviation for the average fuel assembly indicates that coupled feedback interactions are more effectively resolved. Conversely, the model for the hottest fuel assembly may require enhanced mesh refinement, improved coupling algorithms, or higher-order solution methods to mitigate numerical oscillations.

The centerline fuel temperature field exhibits reduced stability when compared to the power field of the hottest fuel assembly, indicating more pronounced delayed numerical effects.

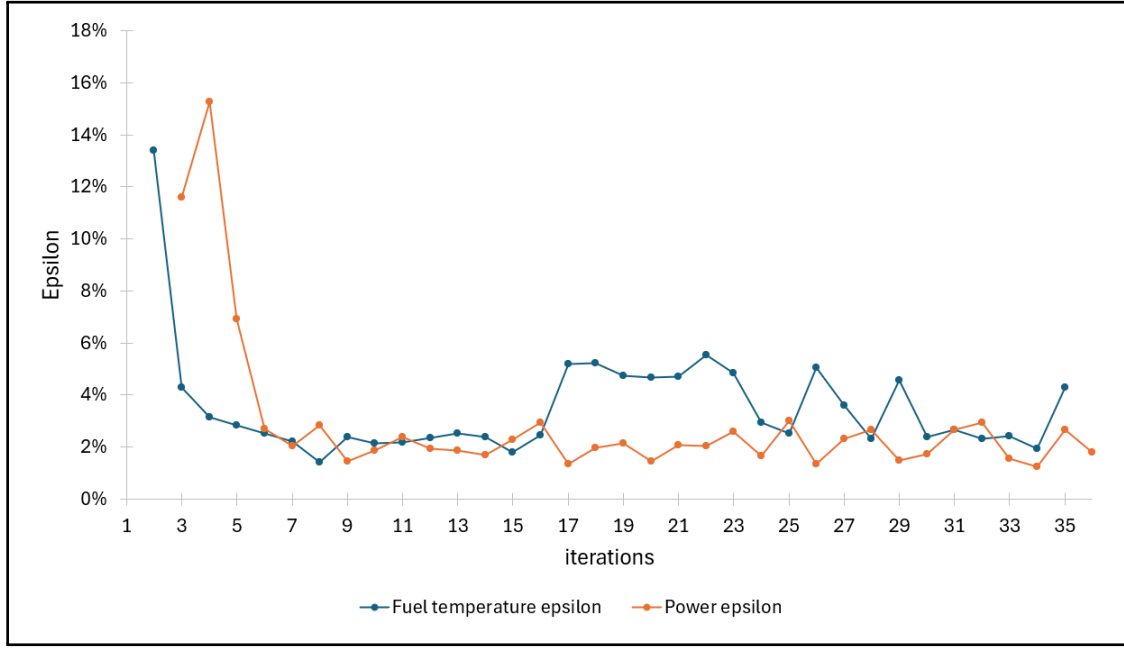


Figure 5.15: Centerline fuel temperature and power variation with Iteration for the hottest fuel assembly

5.3.2.2 Centerline fuel temperature axial profiles

In Iteration 1, the peak centerline fuel temperature for both the hottest fuel assembly (Figure 5.16) and the average fuel assembly (Figure 5.6) provides an initial estimate for numerical coupling. As Iterations progress, the temperature in the hottest fuel assembly deviates from that of the average fuel assembly, attributed to increased local power deposition. In Iteration 2, at axial level 5, the peak temperature reaches 2086.30 K for the hottest fuel assembly, while the average fuel assembly records a temperature of 1698.75 K. Although the overall trend is maintained, the hottest fuel assembly shows a 22.81 % increase in fuel temperature across the axial profile.

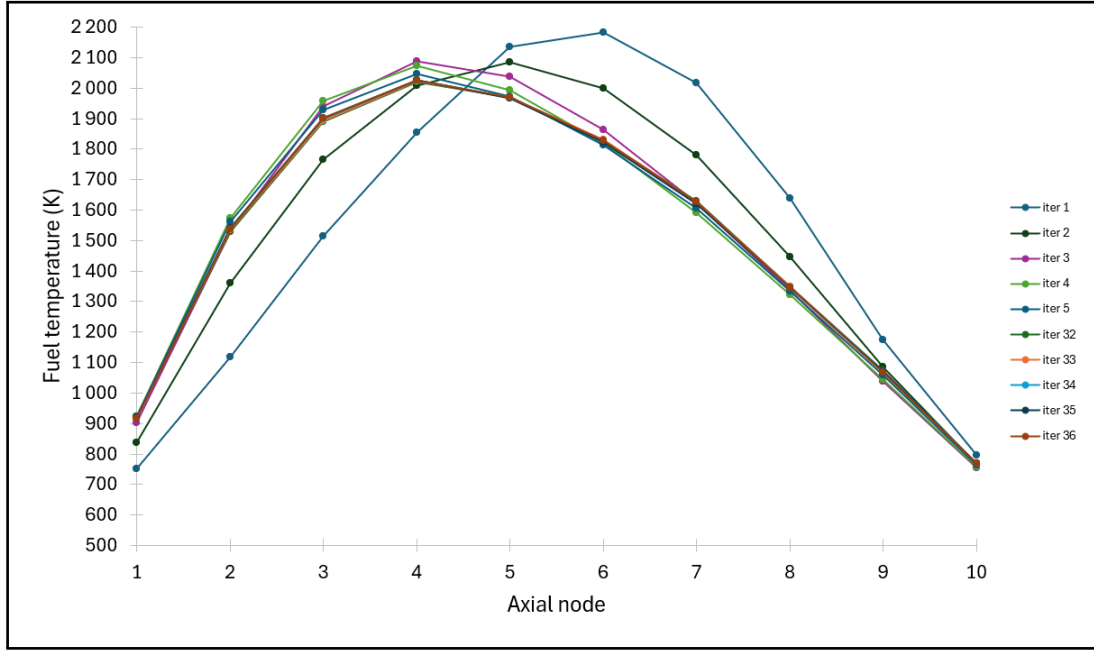
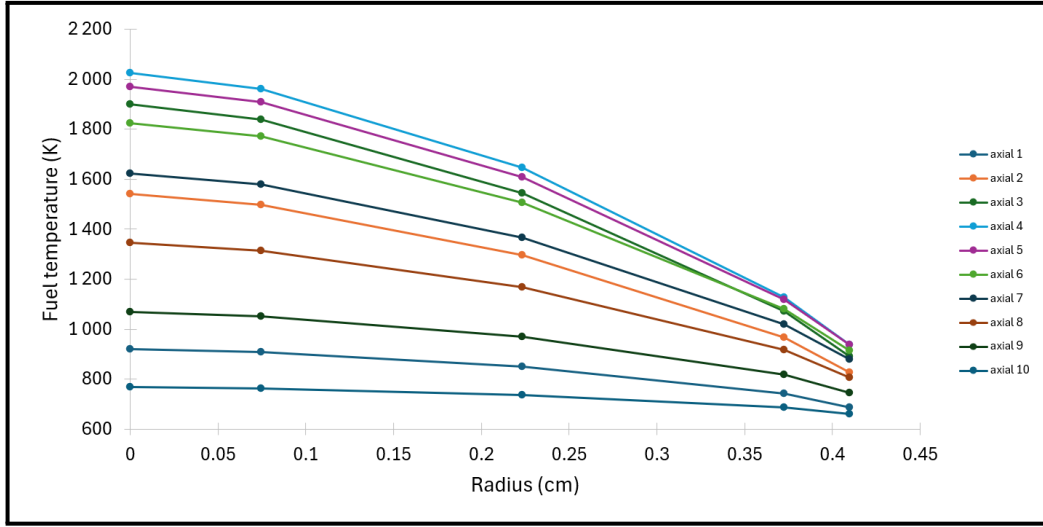


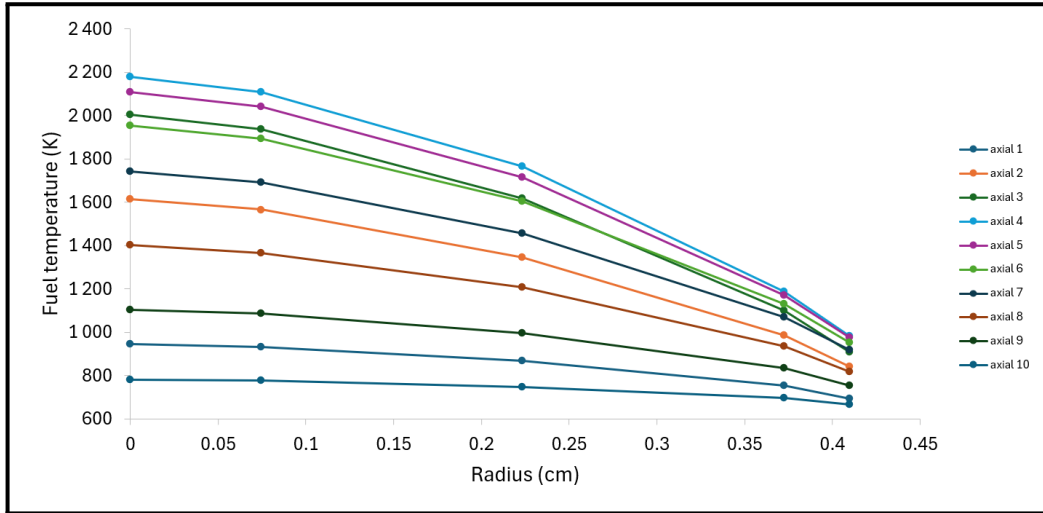
Figure 5.16: Centerline fuel temperature axial profiles for the hottest fuel assembly

5.3.2.3 Fuel temperature radial profiles

The fuel temperature radial profiles for the hottest (Figure 5.17) and average fuel assembly (Figure 5.7) models exhibit a trend of decreasing temperature from the centre outward. In both assemblies, the radial fuel temperature distribution is averaged across all pins of Iteration 34, with pin 213 identified as the hottest pin in the hottest assembly. Both profiles reach a maximum at axial level 4, indicating that the highest thermal conditions occur at this location. Despite similar shapes, temperature values are consistently higher in the hottest fuel assembly model. At axial level 4, the peak fuel temperature for the average pins is 1660.38 K in the average fuel assembly, while in the hottest fuel assembly, it increases to 2025.52 K, representing a 22 % rise. For the hottest pin, the peak fuel temperature rises from 1753.66 K in the average fuel assembly to 2178.22 K in the hottest fuel assembly, reflecting a 24.21 % increase at the same axial level. Although the radial temperature profiles maintain the same overall shape, variations in temperature values can be attributed to localised power-peaking effects. The hottest pin consistently records the highest temperatures, exhibiting a more pronounced thermal gradient across the fuel radius, emphasising the impact of localised heat deposition on fuel performance and safety margins.



(a) Iteration 34 average pin fuel temperature radial profiles



(b) Highest pin fuel temperature radial profile

Figure 5.17: Comparison of fuel radial profiles in the hottest fuel assembly

5.3.3 Coolant temperature axial profiles

This subsection presents results related to the coolant temperature of the hottest fuel assembly model.

Figure 5.18 presents the coolant temperature axial profiles for both the average and hottest assemblies at Iteration 34, where both assemblies experienced convergence. The axial profiles of both the average and hottest assemblies follow similar trends; however, at axial level 10, the hottest assembly exhibits a higher coolant temperature of 595.79 K compared to 590.47 K for the average assembly. The higher coolant temperature in the hottest assembly arises from its greater power output relative to the average assembly. Although both assemblies exhibit the same pin peaking factor, the increased heat generation in the

hottest assembly results in a higher coolant temperature at corresponding axial levels. The deviation in coolant temperature rise for the hottest fuel assembly is 13.03 % from the SAR stated rise, while the average fuel assembly shows a deviation of 26.68 %.

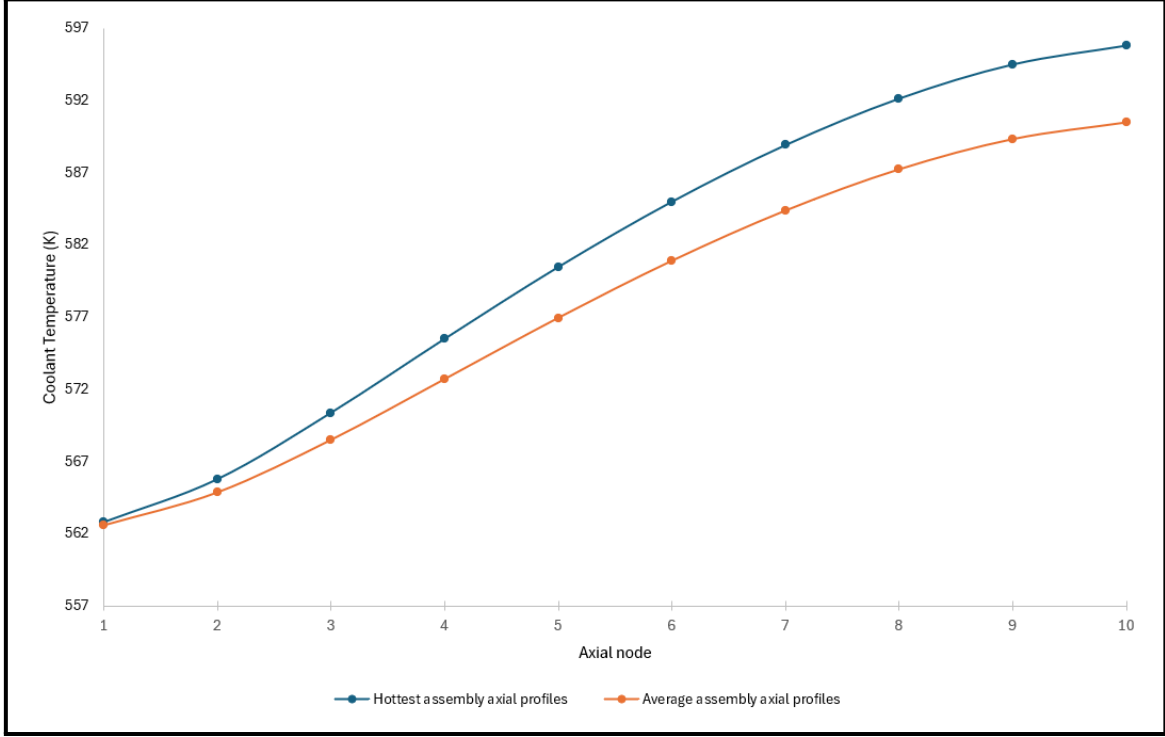


Figure 5.18: Axial coolant temperature profiles for the average and hottest fuel assemblies at Iteration 34 (converged)

5.3.4 Infinite multiplication factor

This subsection presents the results related to the infinite multiplication factor for the hottest fuel assembly model.

5.3.4.1 Infinite multiplication factor vs. Iterations

Figure 5.19 illustrates the infinite multiplication factor as a function of Iterations for the hottest and average fuel assembly. The initial value for the hottest fuel assembly is 1.2974, while the average fuel assembly starts at 1.2977. Both assemblies show a decreasing trend, with the value dropping to 1.2878 by Iteration 4 for the hottest fuel assembly and 1.2942 for the average fuel assembly. Numerical stability and convergence are reached by Iteration 5, with variations of 60 pcm for the hottest fuel assembly and 40 pcm for the average fuel assembly. Epsilon values remain below 0.03 % for both assemblies. The hottest fuel assembly range is consistent with a standard deviation of 26.1 pcm (3 sigmas) obtained from a stand-alone Serpent calculation for the hottest fuel assembly. The hottest fuel assembly stabilises at approximately 1.2889, while the average fuel assembly stabilises at

around 1.2947. The k_{∞} of the average fuel assembly stabilises at a higher value compared to the hottest fuel assembly, which is expected due to the influence of fuel temperature feedback. The higher fuel temperature in the hottest fuel assembly increases the Doppler broadening of resonance absorption in U-238. This phenomenon leads to greater neutron absorption in resonance regions, resulting in a more significant reduction of k_{∞} in the hottest fuel assembly compared to the average fuel assembly, where temperatures are lower.

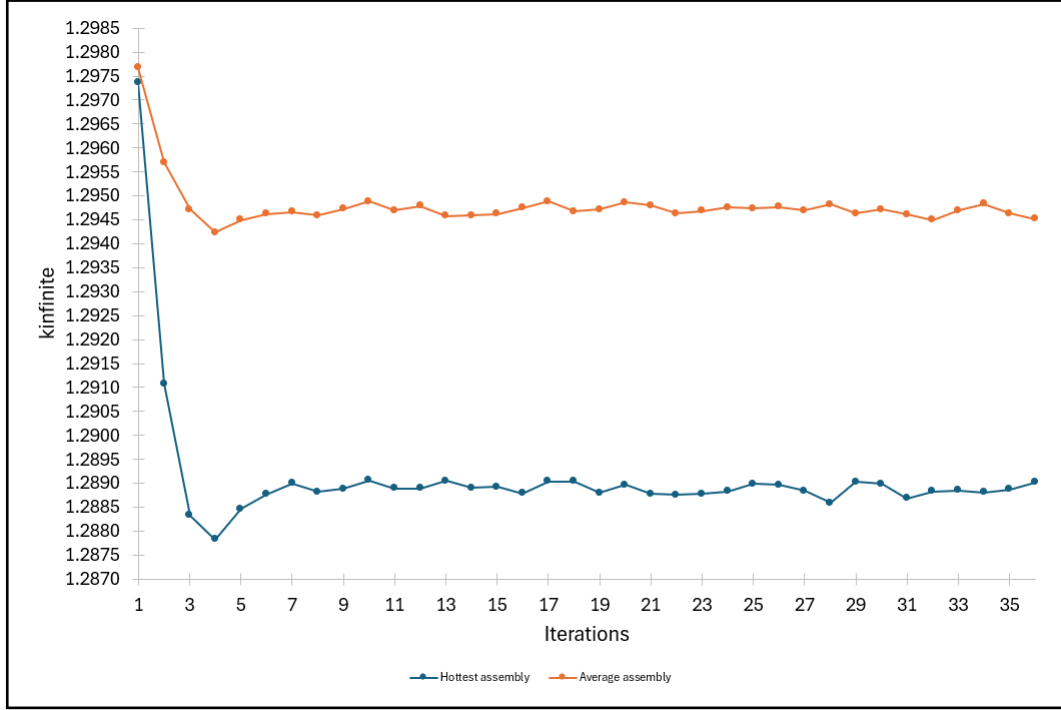


Figure 5.19: Comparison of the infinite multiplication factor vs. Iterations for the hottest and average fuel assembly

5.3.4.2 Variation of infinite multiplication factor and average coolant temperature with Iterations

Figure 5.20 illustrates the comparison of average coolant temperature across Iterations for the hottest assembly, while Figure 5.10 presents the average assembly data. Both plots exhibit similar trends regarding k_{∞} and average coolant temperature. At Iteration 1, the coolant temperature for the hottest fuel assembly is recorded at 579.41 K, while the average fuel assembly coolant temperature is 576.62 K. From Iteration 5 onwards, both plots demonstrate numerical convergence and stability, with the temperature range for the hottest fuel assembly being 0.16 K and for the average fuel assembly, 0.09 K. Notable fluctuations in k_{∞} for the average fuel assembly are noted; however, the narrow range suggests these fluctuations do not indicate divergence. Across the Iterations, the average coolant temperature for the hottest fuel assembly is measured at 581.10 K, reflecting a deviation of 0.57 % from the average fuel assembly's temperature. The standard deviation for the hottest fuel assembly is 0.03 K.

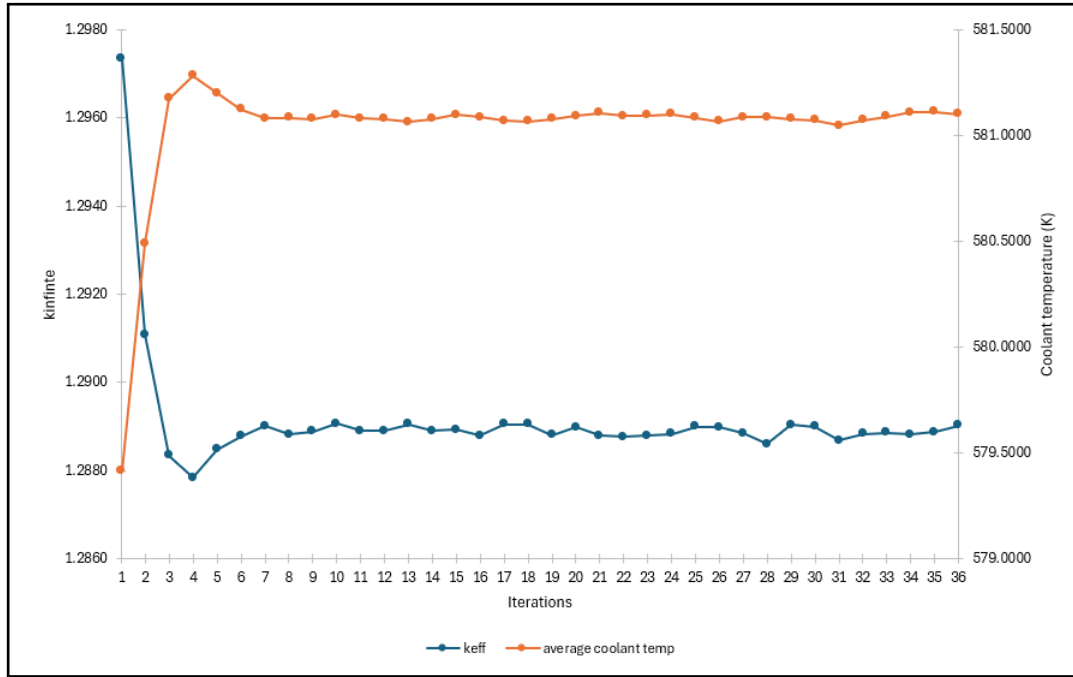


Figure 5.20: Variation of infinite multiplication factor and average coolant temperature with Iterations for the hottest fuel assembly

5.3.4.3 Variation of infinite multiplication factor and average centerline fuel temperature with Iterations

Figure 5.21 presents the variation of the infinite multiplication factor alongside the average and maximum centerline fuel temperatures over Iterations for the hottest assembly and 5.11 for the average assembly. At Iteration 1, the maximum fuel temperature for the hottest fuel assembly is recorded at 1948.09 K, while the average fuel centreline temperature measures 1518.15 K. Conversely, in Iteration 1 for the average fuel assembly, the maximum fuel temperature is 1657.66 K, and the average fuel centreline temperature is 1283.80 K. Numerical stability and convergence are observed beginning at Iteration 5 for both assemblies. The standard deviation of the maximum fuel temperature for the hottest fuel assembly is 10.13 K, with the average temperature standard deviation at 0.65 K. The maximum fuel temperature for the hottest fuel assembly stabilises at 2175.73 K, with the average fuel temperature stabilising at 1498.35 K. Relative to the average assembly, the hottest assembly exhibits a maximum fuel temperature that is 472.59 K higher. This outcome is consistent with expectations, as the hottest assembly possesses greater power.

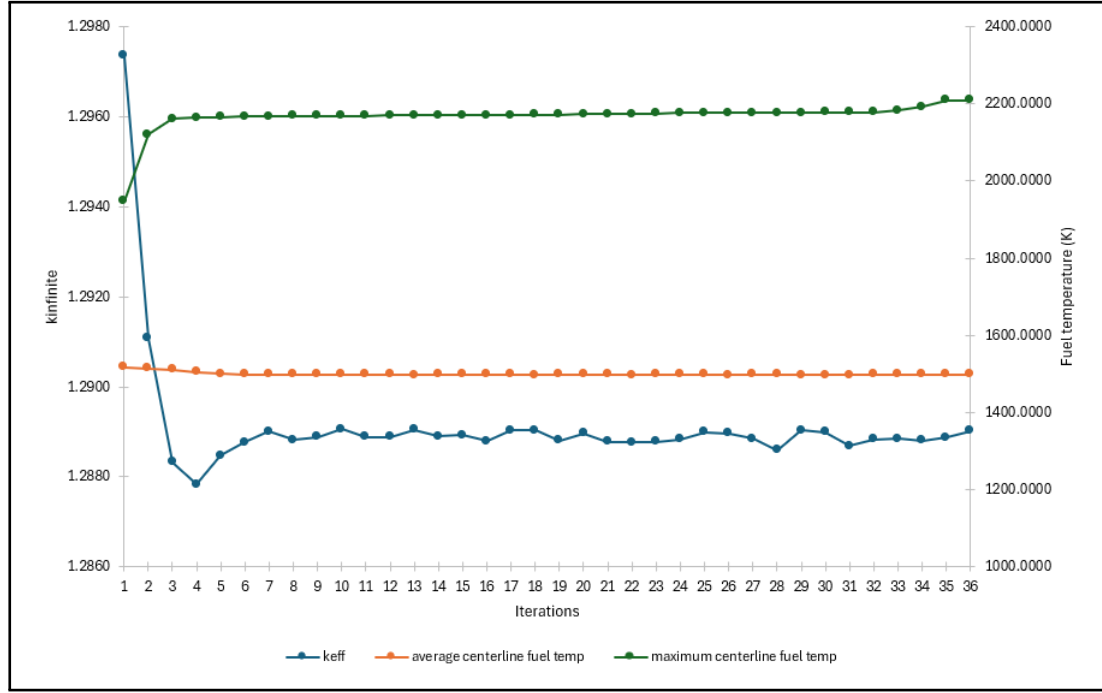


Figure 5.21: Variation of infinite multiplication factor and average centerline fuel temperature with Iterations for the hottest fuel assembly

5.4 Conclusion

The comparison of the two models presented in Table 5.4 indicates that the hottest fuel assembly model exhibits significant fluctuations in fuel temperature and power epsilons, attributed to increased power-dependent feedback mechanisms. In contrast, the average fuel assembly model demonstrates enhanced stability and convergence of the different fields.

The axial and radial profiles of both models indicate effective coupling of the simulations. Consequently, the resulting data is regarded as credible for accurately representing reactor behaviour.

The simulations indicated that the predicted values remained below the fuel centerline temperature and clad outside surface temperature limits outlined in Section 3.5, indicating compliance with safety criteria at steady state.

Aspect	Average Fuel Assembly Model	Hottest Fuel Assembly Model
Power Epsilon vs. Iterations	Converged Iteration is Iteration 34	Converged Iteration is Iteration 34
Power Axial Profiles	Stabilised coupled solution.	Stabilised coupled solution
Fuel Radial Profiles	Experiences peak at radial level 4 for pin average temperatures and for the highest pin temperature, which is pin 205	Experiences peak at radial level 4 for pin average temperatures and for highest pin temperature, which is pin 213
Centerline Fuel Temperature vs. Iterations	Converges by Iteration 4	Instability, no convergence
Centerline Fuel Temperature Axial Profiles	Stable across Iterations	Stable across Iterations
Average Fuel Temperature Radial Profiles	Stable across Iterations	Stable across Iterations
Coolant Temperature Axial Profiles	Stable across Iterations	Stable across Iterations
kinf vs. Iterations	Converges from Iteration 6	Converges from Iteration 5
kinf vs. Average Coolant Temperature	Converges from Iteration 5	Converges from Iteration 7
kinf vs. Average Centerline Fuel Temperature	Converges from Iteration 10	Converges from Iteration 5

Table 5.4: Comparison of the hottest fuel assembly model and the average fuel assembly model

Chapter 6

Summary and recommendations

This study coupled N and TH of the NAPS PWR utilising Serpent and Flownex. This research achieved coupling at the pin-by-pin level for both the hottest fuel assembly and average fuel assembly models. The existing literature lacks a comprehensive study that couples Serpent and Flownex at the pin-by-pin level.

6.1 Full-core NWURCS model

This study modelled the Westinghouse RFA-2 fuel assembly, representing the latest fuel design used at NAPS. A NAPS full-core model developed by Mphofu [106] was modified to incorporate the RFA-2 fuel assembly parameters in accordance with the SAR, rather than the previous LOPAR fuel assembly design parameters utilised in the original model. Following the modification, the updated model was compared against the NWURCS NAPS full-core model by Ringane [105] for verification. The NWURCS model also underwent modifications, with the addition of components such as the upper and lower reflectors, thermal shields, barrel, and baffles to ensure alignment with the SAR. Once the manual and NWURCS full-core models were updated to reflect the SAR, a verification process was conducted. This process was essential to ensure that the models met the specified requirements and performed accurately under predetermined conditions. Upon achieving a k_{eff} difference of 54 pcm between the two models, confidence was established to proceed with the NWURCS model.

The results of the modified NWURCS full-core enabled the initiation of coupling, as Serpent provided the total core power and average fuel assembly power results. However, localised variations in the reactor core resulted in over-predicted power values for the hottest fuel assembly as provided by Serpent. The F_Q computed by Serpent was found to be 1.9307, contributing to the incorrect representation of the hottest fuel assembly. This discrepancy warrants refinement and further investigation in future work. A $F_{N\Delta H}$ value of 1.21, derived from a SAR condition closely resembling the model, was utilised to obtain

the correct power peaking value for the hottest fuel assembly. Coupling procedures were implemented after modifying the Flownex fuel assembly model to specify all necessary parameters and material compositions according to SAR.

6.2 Coupling

External coupling was selected due to the higher computational costs associated with internal coupling, as noted in earlier literature, and the unavailability of the source code. The research coupled N and TH through a serial integration coupling strategy involving the sequential processing of one model while using its outputs as inputs for the subsequent model. A convergence criterion was established for each field prior to coupling, allowing for the determination of when the simulation achieved convergence. Epsilon convergence thresholds were defined at 0.05 % for the k_{∞} field, 0.3 % for the power field, 0.6 % for the coolant temperature field, and 0.3 % for the fuel temperature fields. The convergence criterion for and centerline fuel temperature versus iteration was established at 2 % based on the limitations on further reduction potential. A relaxation factor of 0.5 was applied to the fields of power, coolant temperature, and fuel temperature. The relaxation factor serves to minimise fluctuations between iterations, thus mitigating the risk of divergence linked to significant non-linear changes.

The comparison of the average and hottest fuel assembly model results indicates that both assemblies operate in a supercritical state, as evidenced by their k_{∞} values exceeding 1. This condition is expected under the assumption of negligible leakage and surrounding influences on the assemblies. The hottest fuel assembly model exhibits fluctuations, as indicated by the differences between the mean and standard deviation in fuel temperature and power epsilons. Specifically, there is a power epsilon median difference of 0.09 % and a standard deviation difference of 0.08 % between the power epsilons in the hottest and average fuel assembly. Based on the power epsilon values, Iteration 34 was identified as the converged iteration for both the average and hottest assemblies, each yielding a pin peaking factor of 1.16, defined relative to the assembly-average power. The hottest assembly corresponds to a core-referenced pin peaking factor of 1.40. Furthermore, there is a centerline fuel temperature median difference of 2.10 % and a standard deviation difference of 0.61 % between the power epsilons in the two assemblies. These discrepancies are attributed to increased power-dependent feedback mechanisms. In contrast, the average fuel assembly model displays improved stability and convergence across various fields. However, both models exhibit low power standard deviation and low centerline fuel temperature standard deviation, indicating stability as the values cluster around median measures.

Differences in coolant temperatures were observed between the cool.ifc files and the Flownex output node. This inconsistency may result from uncertainty regarding which tables to use for verification in the SAR and insufficient TH design parameter information pertaining to the RFA-2 fuel assembly. However, the coolant axial temperature data from the cool.ifc

file indicates that the coolant at the top of the core for both models remains below the specified temperature of 600.87 K. The coolant temperature rise deviates by 26.68 % for the average fuel assembly model and 13.03 % for the hottest fuel assembly model, from the rise stated in the SAR. Additionally, the fuel temperature at the top of the core in the hottest fuel assembly model is 75.01 % lower than the fuel melting temperature noted in the SAR, thus confirming that the fuel remains significantly below critical failure limits. These findings suggest effective N/TH numerical coupling and confirm that both models maintain compliance with established safety limits.

6.3 Recommendations for future work

1. Data extraction was performed manually using MATLAB; however, the future development and implementation of automated MATLAB scripts is recommended to enhance efficiency.
2. The manual entry of the user password for each job submission contributed to the prolonged time between iterations. This issue can be mitigated in the future by employing Secure Shell (SSH) key-based authentication, eliminating the need for password entry each time.
3. A future recommendation for improving data transfer efficiency between the two solvers is to adopt binary formats such as Hierarchical Data Format 5 (HDF5), which are designed for high-speed performance rather than text-based file transfer.
4. Investigate alternative relaxation factors to the value of 0.5, as different factors may improve numerical stability or accelerate convergence.
5. This model is fully one-dimensional; however, in reality, cross-flow occurs and should be incorporated in future work.
6. An error was encountered in NWURCS when Uranium-234 was included in the fuel composition, resulting in a bug. This was temporarily resolved by excluding the isotope; however, future work should address this issue to allow for accurate modelling of U-234.
7. The SAR specified that the top and bottom reflectors consist of water and steel, but did not provide exact composition details. A secondary source indicated a 50/50 mixture without specifying whether it referred to weight or atomic percent. This study assumed a 50/50 weight percent based on convention. Future work should seek more definitive data to improve model accuracy.
8. Stainless steel was initially used for the RPV, but examiner feedback indicated that low-alloy steel would have been more appropriate. Although this is unlikely to impact the coupling results significantly, future models should use the correct material.
9. For future work, it is recommended to investigate and analyse the causes of deviation in outlet temperature between the coupled results and the SAR.

10. Finally, due to time constraints and limited geometric data, the reactor shield was modelled as circumferential based on available references. While a more detailed geometry could enhance accuracy, it is not expected to affect neutronic results. Future work may benefit from a more refined shield representation.

Appendix A

Serpent full-core input file

The full Serpent input file used for this study is archived and accessible on Zenodo: <https://doi.org/10.5281/zenodo.16271919>

Appendix B

MATLAB code for assembly power analysis

The following MATLAB script was used to process Serpent output and analyse the core's assembly power distribution.

```
1 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
2 %% Initial checking and pre-processing %%
3 %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
4
5 % Define the file path
6 file_path = 'C:\\Users\\palpr\\OneDrive - North-West University\\
7             Masters\\nwurcsfullcoredet141024\\serpent_det0.m';
8
9 % Check that the detector file exists
10 if exist(file_path, 'file') ~= 2
11     disp(['Could not find serpent_det0.m from the specified path: ',
12          file_path]);
13     return;
14 end
15
16 % Run the detector output file to bring the results to workspace
17 try
18     run(file_path);
19 catch ME
20     disp(['Error running serpent_det0.m: ', ME.message]);
21     return;
22 end
23
24 % Check that the detector outputs exist for assembly powers
25 if ~exist('DETassemblypowers', 'var')
26     disp('Could not find results for assembly powers from the detector
27         file (maybe misspelled detector name?). Cannot do analysis.');
```

[illegible]

```

66 % Plotting the assembly power distribution
67 figure('visible', 'off');
68 imagesc(1:core_size_x, 1:core_size_y, assembly_powers_grid); % Use
    integer grid for plot
69 colormap(jet);
70
71 % Add a colorbar
72 cb = colorbar();
73 set(cb, 'FontSize', 16);
74 title(cb, 'Linear power (W/cm)', 'FontSize', 14);
75
76 % Add title and labels
77 title('Assembly Power Distribution', 'FontSize', 14, 'FontWeight', '
    bold', 'Interpreter', 'none');
78 xlabel('X-coordinate (assembly index)');
79 ylabel('Y-coordinate (assembly index)', 'FontSize', 12);
80
81 % Mark the hottest assembly on the plot
82 hold on;
83 plot(col, row, 'rx', 'MarkerSize', 10, 'LineWidth', 2); % Red cross to
    indicate hottest assembly
84 hold off;
85
86 % Adjust y-axis tick label font size
87 set(gca, 'FontSize', 10);
88
89 % Calculate the average assembly power
90 num_assemblies = 157; % Number of assemblies in the core
91 average_power = total_core_power / num_assemblies; % Mean of all
    assembly powers based on total core power
92
93 % Calculate the assembly peaking value
94 assembly_peaking_value = hottest_assembly_power / average_power; %
    Ratio of hottest to average
95
96 % Display additional information
97 disp(['Average Assembly Power: ', num2str(average_power), ' W']);
98 disp(['Assembly Peaking Value: ', num2str(assembly_peaking_value)]);
99
100 % Save the figure
101 print -dpng AssemblyPowersWithHottest.png;
102
103 % Close the figure
104 close(gcf);

```

Appendix C

Figures from external references

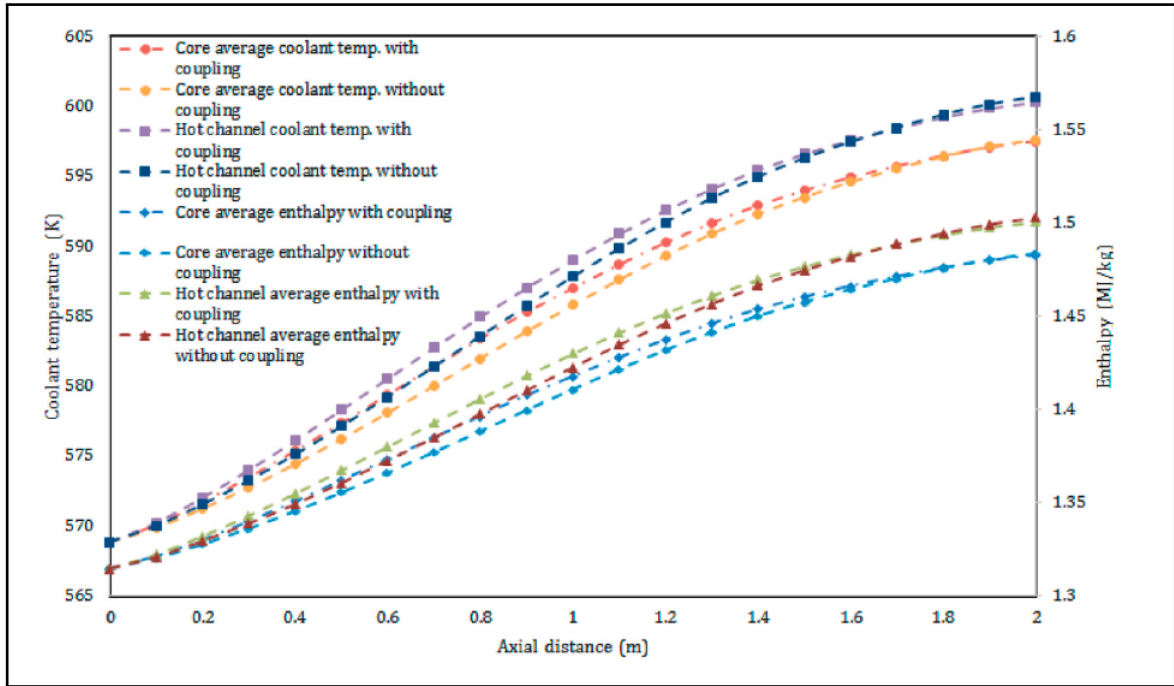


Figure C.1: Average thermal-hydraulics parameters of the SMART reactor core in the state with and without the co-coupling.

[45]

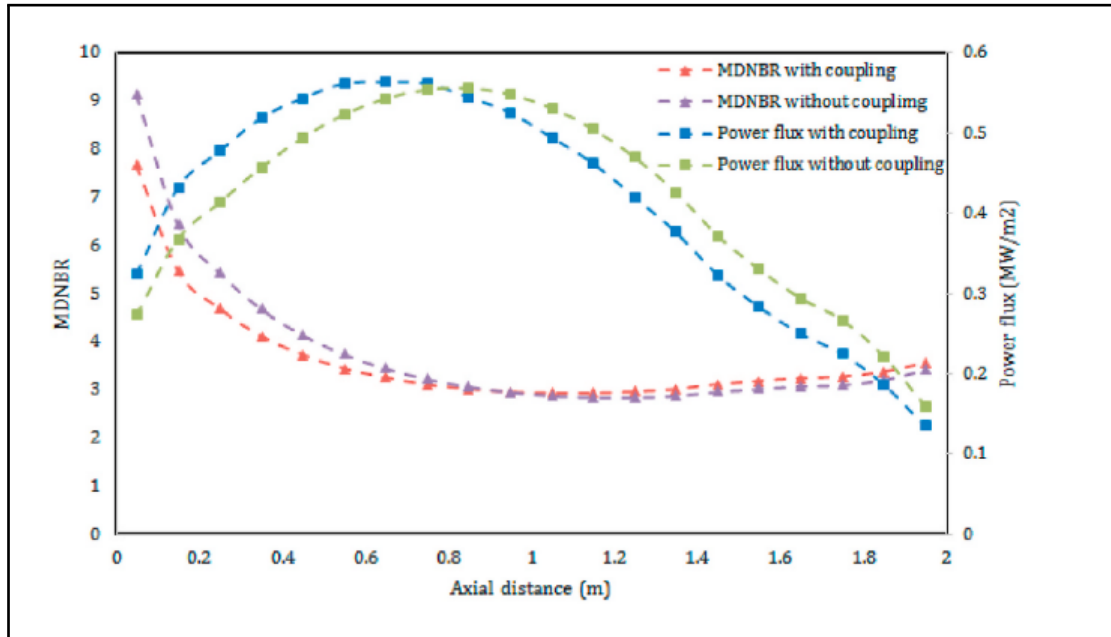


Figure C.2: MDNBR and core power flux of SMART reactor with and without the coupling process.

[45]

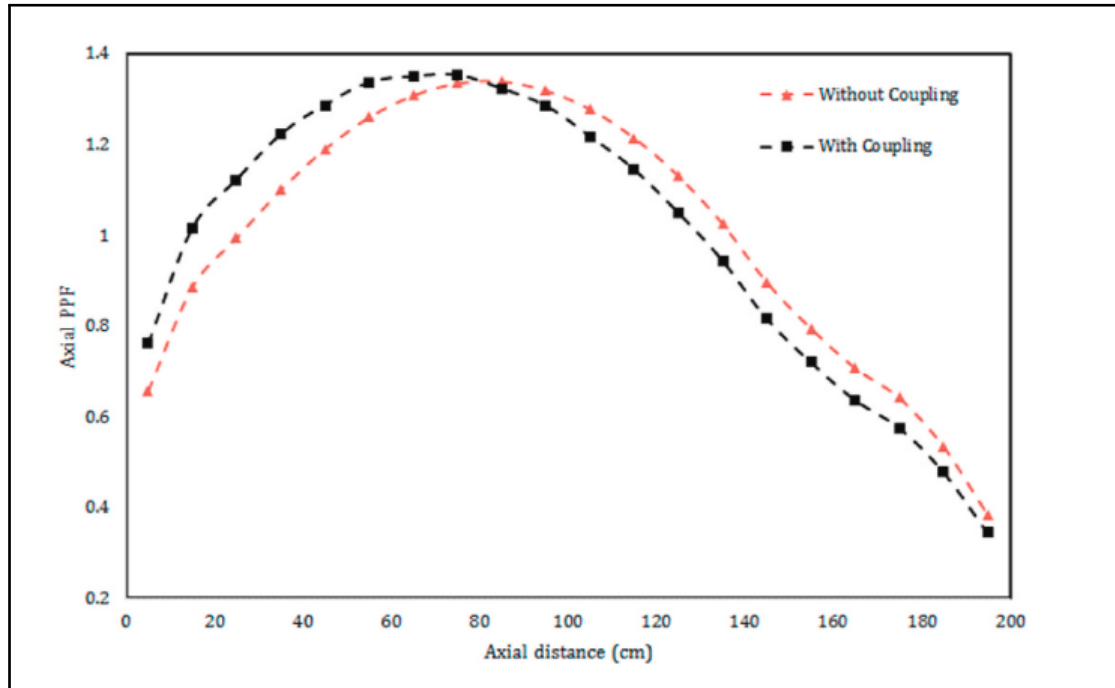


Figure C.3: SMART reactor peak power factor with and without code coupling process.

[45]

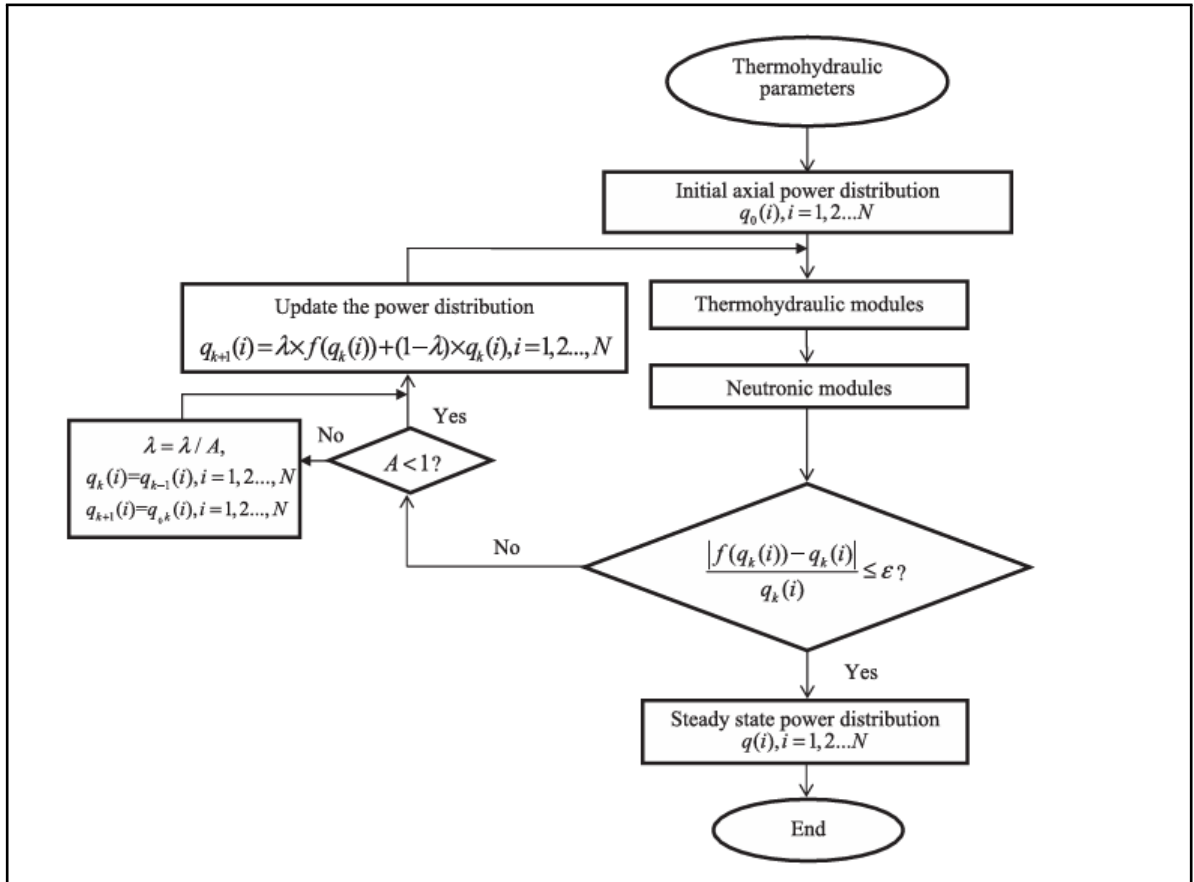


Figure C.4: Calculation process of N/TH coupling (self-adaptive relaxation factor)

[60]

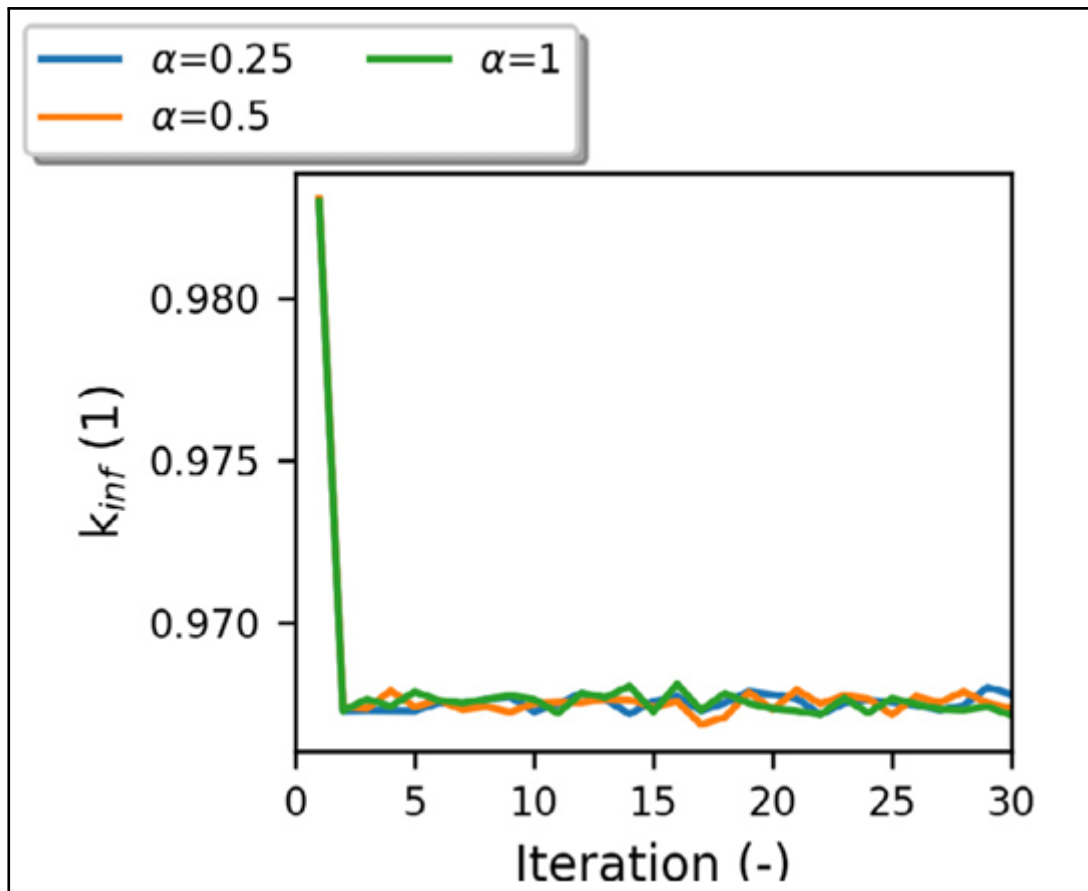


Figure C.5: Multiplication factor during coupled iterations relaxation factor study
[61]

Revision 56--Updated Online 09/30/20		NAPS UFSAR	4.4-59
Table 4.4-3			
THERMAL HYDRAULIC DESIGN PARAMETERS OF THE WESTINGHOUSE 17 X 17 RFA-2 FUEL			
Reactor Coolant System			
Rated Thermal Power		2940 MWt	
Heat Generated in Fuel		97.4%	
Nominal System Pressure		2250 psia	
Coolant Flow			
Thermal Design Flow		278,400 gpm	
Minimum Measured Flow		295,000 gpm	
Mechanical Design Flow		315,600 gpm	
Coolant Temperature			
Nominal inlet		551.7°F	
Average rise in vessel		70.2°F	
Average in vessel		586.8 °F	
Heat Transfer			
Average heat flux		202,000 Btu/hr-ft ²	
Average linear heat rate		5.80 kW/ft	

Figure C.6: Thermal hydraulic design parameters

[1]

Appendix D

Calculated Material Compositions

Table D.1: Calculation of ZIRLO Isotopic Composition

Isotope	Abundance	Atomic Mass (u)	Weighted Atomic Mass	Avg.	Mass Density	Final Composition
Zirconium						
Zirconium-90	5.1450E-01	89.904704	91.223647		7.6808E-23	5.0295E-01
Zirconium-91	1.1220E-01	90.905645			1.6936E-23	1.0968E-01
Zirconium-92	1.7150E-01	91.905040			2.6172E-23	1.6765E-01
Zirconium-94	1.7380E-01	93.906316			2.7101E-23	1.6990E-01
Zirconium-96	2.8000E-02	95.908276			4.4592E-24	2.7371E-02
Iron						
Iron-54	5.8450E-02	53.939615	55.84515		5.2352E-24	5.8450E-05
Iron-56	9.1754E-01	55.934942			8.5221E-23	9.1754E-04
Iron-57	2.1190E-02	56.935399			2.0033E-24	2.1190E-05
Iron-58	2.8200E-03	57.933280			2.7128E-25	2.8200E-06
Tin						
Tin-112	9.7000E-03	112.904704	118.7318		1.8185E-24	9.7000E-05
Tin-114	6.6000E-03	113.902784			1.2483E-24	6.6000E-05
Tin-115	3.4000E-03	114.903348			6.4871E-25	3.4000E-05
Tin-116	1.4540E-01	115.901747			2.7983E-23	1.4540E-03
Tin-117	7.6800E-02	116.902956			1.4908E-23	7.6800E-04
Tin-118	2.4220E-01	117.901609			4.7417E-23	2.4220E-03
Tin-119	8.5900E-02	118.903311			1.6960E-23	8.5900E-04
Tin-120	3.2590E-01	119.902199			6.4886E-23	3.2580E-03
Tin-122	4.6300E-02	121.903440			9.3721E-24	4.6300E-04
Tin-124	5.7900E-02	123.905274			1.1913E-23	5.7900E-04
Chromium						
Chromium-50	4.3000E-02	49.946	51.94528		3.5662E-24	2.0422E-06
Chromium-52	8.3700E-01	51.9405			7.2189E-23	3.9381E-05
Chromium-53	9.5500E-02	52.9407			8.3952E-24	4.4655E-06
Chromium-54	2.3500E-02	53.9389			2.1048E-24	1.1115E-06
Niobium						
Niobium-93	1.0000E-02	92.906378	92.906378		9.2906E-24	1.0000E-02
Oxygen						
Oxygen-16	9.9790E-01	15.994914	16.999131		1.5958E-23	9.9790E-01
Oxygen-17	3.7990E-04	16.999132			6.0885E-27	3.7990E-04
Oxygen-18	2.0000E-03	17.999159			3.1735E-26	2.0000E-03

Appendix E

ZIRLO material properties

E.1 Corrosion resistance

ZIRLO demonstrates lower corrosion rates compared to Zircaloy-4, especially at high burnup levels, contributing to enhanced fuel assembly longevity and reliability [110]. The reduced oxide layer thickness on ZIRLO cladding mitigates nodular corrosion and Hydrogen embrittlement, maintaining structural integrity under operational conditions [111].

E.2 Dimensional stability

ZIRLO shows enhanced dimensional stability during extended irradiation compared to Zircaloy-4, resulting in decreased operational disruptions and increased safety margins in reactor operation [110].

E.3 Thermal properties

Zircalloy has a melting temperature between approximately 2,123 K and 2,128 K [112]. The specific melting point of its base material, Zirlo, is not detailed in existing literature. However, research indicates that Cr-coated Zirlo undergoes eutectoid melting at 1,589.15 K. This phenomenon is attributed to the diffusion of chromium and the formation of β -phase under thermal stress [113]. This difference affects the materials' specific heat and thermal response during transient conditions, resulting in a performance profile for ZIRLO during temperature excursions [114].

E.4 Reduced Hydrogen generation

The corrosion rates of ZIRLO are lower, resulting in reduced Hydrogen generation in the cladding, which is significant for mitigating embrittlement and potential failure modes [111].

E.5 Operational flexibility

ZIRLO shows improved thermal and mechanical properties that enhance operational flexibility under various reactor conditions, contributing to reactor safety and efficiency [110].

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