

Neutronic analysis of selected fuel assemblies of the MIT BEAVRS benchmark using HEADE collision probability code

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DECLARATION OF AUTHOR

To the best knowledge of the author, this work represents the first verification of the HEADE collision probability code using the MIT BEAVRS benchmark. The author hereby confirms that where published work of others was consulted, it is clearly acknowledged and the source is always given in this dissertation.

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Date: May 2019

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ABSTRACT

Neutronic models for fresh core fuel assemblies of the MIT BEAVRS benchmark are developed using the HEADE collision probability code which is a module of the OSCAR-4 code used for research reactor calculations. This research study is based on the MIT BEAVRS benchmark, which is a specification of a Pressurized Water Reactor (PWR). The neutronics models are performed at 300K, assuming the use of fresh fuel as one state of the BEAVERS benchmark. Parameters such as the k_{inf} , power profiles, flux profiles and group constants were evaluated for selected fuel assemblies taken from the MIT BEAVRS benchmark reactor core. In this study, the applicability of the HEADE collision probability code to a PWR calculation is evaluated. The Serpent code was used as a reference code for selected cases, in order to verify HEADE in this study. The results obtained from the HEADE and Serpent codes for various models were investigated and compared and are presented in this dissertation. The behaviour of the results obtained, confirm that the HEADE code can be used for PWR calculations for the cases considered in this study except for those in which spacer grids were included.

Keywords: HEADE, BEAVRS, neutronics, infinite neutron multiplication factor ($k_{infinity}$), power, flux, group constants.

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TABLE OF CONTENTS

DECLARATION OF AUTHOR.....	i
ABSTRACT	ii
ACKNOWLEDGEMENTS	iii
LIST OF TABLES	vi
LIST OF FIGURES	vii
LIST OF ACRONYMS.....	viii
CHAPTER 1 BACKGROUND AND OVERVIEW	1
1.1 Introduction	1
1.2 Motivation for Research	4
1.3 Problem Statement	5
1.4 Objectives	5
1.5 Organization of Dissertation	6
CHAPTER 2 LITERATURE STUDY	7
2.1 The Pressurized Water Reactor	7
2.1.1 Reactor core	8
2.1.2 Spacer grid.....	9
2.2 BEAVRS Benchmark Overview	10
2.3 Description of the Fuel Assemblies Selected from the BEAVRS Benchmark.....	12
2.4 Review of Studies Involving the MIT BEAVRS Benchmark	16
2.5 Computer Codes Used in this Study	17
2.5.1 HEADE collision probability code	17
2.5.2 Serpent Monte Carlo code	19
CHAPTER 3 THEORY	20
3.1 Neutron Reactions	20
3.1.1 Scattering of neutrons	20
3.1.2 Nuclear fission.....	21
3.2 Nuclear Fission Chain Reaction.....	21
3.3 Neutron Flux.....	22
3.4 Reaction Rate and Cross-Section	22
3.5 Neutron Transport Equation	23
3.6 Stochastic Methods Used to Solve Neutron Transport	24
3.7 Reactor Calculation Strategy	27
3.8 Group Constants.....	29
3.9 Burn-Up	29

CHAPTER 4 METHODOLOGY	33
4.1 Development of the HEADE and the Serpent Models for the Standard Fuel Assembly.....	33
4.2 Burn-Up	35
4.3 Adding a Spacer Grid to a Fuel Assembly	35
4.4 Changing Enrichment.....	37
4.5 Adding Burnable Poison, Control Rods, Instrument Pin	38
CHAPTER 5 RESULTS	40
5.1 Burn-Up	40
5.1.1 Multiplication factor.....	40
5.1.2 Group constants.....	42
5.1.3 Power	44
5.2 Additional Parameters Obtained from HEADE.....	46
5.3 Adding a Spacer Grid to a Fuel Assembly Model – Results.....	50
5.4 Varying Enrichment.....	54
5.4.1 Infinite multiplication factor (k_{inf})	54
5.4.2 Group constants.....	54
5.4.2.1 Absorption cross-section (Σ_{abs}):.....	55
5.4.2.2 Fission cross-section (Σ_f):	55
5.4.2.3 Diffusion coefficient (D):	55
5.4.3 Power profiles	55
5.5 Instrument Pin, Burnable Poison and Control Rods	56
CHAPTER 6 CONCLUSIONS AND RECOMMENDATIONS.....	61
6.1 Conclusion.....	61
6.2 Recommendations for Future Studies	62
REFERENCES	64
APPENDIX A: MATERIAL DEFINITION OF MATERIALS USED IN THE MODELS.....	67
APPENDIX B: BURN-UP RESULTS (HEADE).....	71
APPENDIX C: HEADE V/S SERPENT RESULTS	73

LIST OF TABLES

Table 2-1: Fuel assembly parameters as given in the BEAVRS handbook	16
Table 4-1: Fuel assemblies observed during spacer grid investigation	37
Table 5-1: Comparison of HEADE and Serpent group constants	40
Table 5-2: Comparison of HEADE and Serpent fuel power maps	45
Table 5-3: k_{inf} for fuel assemblies observed during spacer grid investigation	51
Table 5-4: Group constants for the standard fuel assembly with spacer grid and one without	52
Table 5-5: HEADE and Serpent group constants for the fuel assembly with spacer grids	53
Table 5-6: Fuel assemblies with 1.6 %, 2.4 % and 3.1 % fuel enrichment	54
Table 5-7: 1/8 of the power map of direct power for the fuel assemblies with varying fuel enrichment	56
Table 5-8: 1.6 % enriched fuel assemblies. Empty guide tubes, burnable poison, control rods, instrument tube	57
Table 5-9: Power distribution for 1/8 of the fuel assembly	59

LIST OF FIGURES

Figure 2-1: PWR two-coolant steam cycle (USNRC, 2016)	7
Figure 2-2: Schematic diagram of a typical PWR core (EIA, 2015)	8
Figure 2-3: Fuel assembly for a pressurized water reactor (Westinghouse, 1984)	9
Figure 2-4: PWR spacer grid (Buongiorno, 2010)	10
Figure 2-5: Layout of fuel assemblies showing enrichment loading pattern and burnable absorber positions in cycle 1 (Horelik & Herman, 2013)	11
Figure 2-6: Fuel assembly guide tube locations. Blank denotes fuel rods, G denotes a guide tube location, and I denotes a guide tube position that might contain an instrument tube (Horelik & Herman, 2013)	12
Figure 2-7: The 12BA burnable absorber configuration. Blank denotes fuel rods, G denotes a guide tube location, B denotes a burnable absorber rod, and I denotes a guide tube that might contain an instrument tube (Horelik & Herman, 2013)	13
Figure 2-8: Fuel pin diagram and the radii	13
Figure 2-9: Empty guide tube diagram and the radii	14
Figure 2-10: Control rod pin geometry	14
Figure 2-11: Instrument tube pin geometry	15
Figure 2-12: Burnable poison above dashpot	15
Figure 3-1: Neutron behaviour in a nuclear reactor	21
Figure 4-1: A HEADE geometry and materials outline for the 17 x 17 fuel assembly	34
Figure 4-2: Fuel pin-cell geometry for the Zircaloy intermediate spacer grid	36
Figure 5-1: Comparison of HEADE and Serpent k-infinity	41
Figure 5-2: Absorption cross-section versus burn-up	43
Figure 5-3: U-235 depletion during burn-up	44
Figure 5-4: Power profile for the standard fuel assembly	46
Figure 5-5: Change in concentration of uranium isotopes versus burn-up	46
Figure 5-6: Build-up of Plutonium isotopes	47
Figure 5-7: Samarium-149 concentration versus burn-up	48
Figure 5-8: Xenon-135 concentration versus burn-up time (540 days)	49
Figure 5-9: Xenon-135 concentration versus burn-up (100MWD/tU)	49
Figure 5-10: Power profiles for row 1 in Table 5-7	56
Figure 5-11: Power profiles for empty GT versus burnable poison	60
Figure 5-12: Power profiles for control rods versus empty GT	60

LIST OF ACRONYMS

<i>Acronym</i>	<i>Meaning</i>
BEAVRS	Benchmark for Evaluation And Validation of Reactor Simulations
BWR	Boiling Water Reactor
CORANA	CORe ANALysis
CROGEN	CROss-section GENeration
CROLIN	CROss-section LINKer
DoE	Department of Energy
EPR	European Pressurized Reactor
GCR	Gas Cooled Reactors
HEADE	HEterogeneous Assembly DEpletion code
HFR	High Flux Reactor
HOR	Hoger Onderwijs Reactor
HTGR	High Temperature Gas-cooled Reactor
HZP	Hot Zero Power
IAEA	International Atomic Energy Agency
LWR	Light Water Reactor
MGRAC	Multi-Group Reactor Analysis Code
MIT	Massachusetts Institute of Technology
NNR	National Nuclear Regulator
NWU	North West University
PWR	Pressurized Water Reactor
OSCAR-4	Overall System for the Calculation of Reactors, generation 4
RRT	Radiation and Reactor Theory
RMC	Continuous-energy Reactor Monte Carlo neutron and photon transport code
SAFARI-1	South African Fundamental Atomic Reactor Installation-1
SMNE	School of Mechanical and Nuclear Engineering
VVER	Water-Water Energetic Reactor
WNA	World Nuclear Association

CHAPTER 1 BACKGROUND AND OVERVIEW

1.1 Introduction

As on 31 December 2016, there were 448 power reactor units in operation worldwide, supplying about 391.1 GWe of electricity (IAEA, 2017). Amongst these 448 power reactors, 289 were pressurized water reactors (PWRs) producing 271.9 GWe, 78 were Boiling Water Reactors (BWRs) producing 75.3 GWe and 14 were Gas Cooled Reactors (GCR) producing 7.7 GWe. As in December 2016, 61 power reactors were under construction with a projected net capacity of 61.2 GWe. Out of the 61 power reactors that were under construction, 51 were PWRs and 4 were BWRs (IAEA, 2017). It is also stated that during 2016, construction started on 3 reactors, 11 reactors were newly connected to the grid and the status in December 2016 was that 80 power reactors were known to be planned. This shows the role that power reactors play and will continue to play in the production of electricity in the world. It has to be ensured that these power reactors are designed and operated safely.

The safety analysis (or assessment) of the operation of nuclear power plants plays an essential role in ensuring their safety in the design period and over long term operation. According to the IAEA (IAEA, 2009), safety analyses are analytical evaluations of physical phenomena occurring at nuclear power plants. They are made for the purpose of demonstrating that safety requirements, such as the requirement for ensuring the integrity of barriers against the release of radioactive material and various other acceptance criteria, are met for all postulated initiating events that could occur over a broad range of operational states, including different levels of availability of the safety systems.

Safety analysis of nuclear reactor systems therefore remains critical to assure the public of the safety and reliability of nuclear power plants. Safety analysis is also critical in aiding countries to make decisions on the type of reactor systems to be built and also to incorporate the lessons from nuclear accidents into safety analysis for added safety assurance. One way safety analyses are achieved is through the performance of reactor calculations.

Reactor calculations, performed using various codes (neutronic codes, thermal hydraulic codes, etc.), are required for predicting and evaluating reactor performance parameters related to reactor utilization and reactor safety assessment. Neutronic calculations can be classified as deterministic or stochastic. For deterministic calculations, once the cross-sections have been processed, the calculations can be performed in two steps, that is, the two-dimensional (2-D) lattice calculation in an infinite environment, performed by the deterministic lattice physics codes, for generating few-group homogenized cross-section and a three-dimensional (3-D) full-core calculation performed by, for example, nodal diffusion codes.

Lattice physics codes perform a series of detailed neutron transport calculations for individual types of fuel assemblies. Each fuel assembly can be divided into several axial zones, with different materials present, and also varying uranium enrichment or burnable absorber content. For each such unique fuel assembly lattice segment, detailed calculations are performed to obtain spatially homogenized and energy collapsed cross-sections. In more sophisticated models, the fuel assembly can also be discretized with respect to the radial (x-y) plane.

Lattice codes compute accurate flux distributions for a detailed representation of a given geometry. The results obtained are then collapsed into a few energy groups and homogenized over the considered volume, and ultimately used as input to the 3-D full core codes (Luszczek, 2015). Examples of the deterministic lattice physics codes are HEADE (Müller, et al., 1-6 05 1994), CASMO-5 (Taforeau & Salino, 2016), HELIOS (Crawford, et al., 2012), CONDOR (Ferraro & Villarino, 2011) and NEWT (DeHart, 2006).

The 3-D full core codes typically divide the reactor core into a number of homogeneous nodes. In such cases, homogeneity means that within a node, neutronic properties, such as the macroscopic cross-sections, are treated as constant over the entire node and are normally obtained from the lattice calculations performed on each node as discussed in the preceding paragraphs. Examples of the 3-D nodal codes are MGRAC (Müller, et al., 1-6 05 1994), SIMULATE-3 (Taforeau & Salino, 2016), PANTHER (Aoki, et al., 2012) and NESTLE (Turinsky, 1994).

Lattice physics codes are benchmarked and validated against either some experimental data, reference Monte Carlo calculations e.g. MCNP, Serpent, TRIPOLLI or other already

verified codes. These activities are required to ensure that the numerical methods and physical approximations implemented in each of the lattice physics codes are accurately accounted for. In this project, the lattice physics code of interest is the HEADE collision probability code which has been extensively used to model the research reactors' plate-type fuel assemblies, but not for PWR pin-type assemblies. In this context, the capabilities of the HEADE code to model PWR pin-type assemblies will be tested on the MIT BEAVRS (Benchmark for Evaluation and Validation of Reactor Simulation) benchmark.

There is only one nuclear power plant in South Africa, namely the Koeberg nuclear power plant, which is also the only one on the African continent. The Koeberg nuclear power plant is owned and operated by the country's only national electricity supplier, Eskom and was commissioned in 1984. The Koeberg nuclear power plant has two pressurized water reactors, each capable of delivering 930 MWe to the grid. Two of the computer codes used at the Koeberg Nuclear Power Plant is SCIENCE and ROSA (Kesonk, 2016). These codes are proprietary and access to the theory and validation of these codes is restricted.

There are growing energy needs in South Africa; these are driven mainly by amongst others: an ageing energy infrastructure, and an energy-intensive socio-economic development agenda that demands major infrastructural development and industrialization programmes. The level of electrification in South Africa presently is too low and a gap of about 90 TWe.h exists between supply and demand (Van Wyk, 2013). In order to address this, the South African government, through the Ministry of Energy, has approved the Integrated Resource Plan (IRP) 2010–2030 (DoE, 2013) in 2011. This plan projects South Africa's electricity supply and demand for a period of 20-years and forecasts that in 20 years' time about 42 % of electricity generated in South Africa will have to come from renewable resources. It provides for the incorporation of 9.6 GWe of nuclear power and 17.8 GWe of renewable energy by 2030. A nuclear fleet, with a total output of 9.6 GWe, instead of one or two nuclear units have been opted for in this plan (Van Wyk, 2013). The IRP is since under revision, and the finalization of the new revision is expected in 2018 (DoE, 2016).

The strongest recent indication of the South African government's intention to pursue nuclear energy actively was the signing of a series of agreements with countries to advance prospects of building up to 9.6 GWe of nuclear capacity by 2030 (WNA, 2016). This is also indicated by Eskom's submission of site licence applications to the National

Nuclear Regulator (NNR) for both Thyspunt and Duynefontein to construct and operate multiple nuclear installations and associated auxiliary nuclear installations.

With this possible expansion in mind and hence possible procurement of nuclear power plants by the South African government, it is necessary that the South African nuclear industry has the expertise and capabilities necessary in modelling power reactors and validation of the candidate neutronics codes together with other codes for the proposed nuclear power plants. The HEADE lattice code could be one such candidate and thus its capabilities to model PWR type assemblies is the main aim of this study.

1.2 Motivation for Research

In accordance with the IRP 2010-2030, the NRF-funded SARCHI Research Chair in Nuclear Engineering, within the School of Mechanical and Nuclear Engineering at the North-West University, initiated research studies focused on Light Water Reactor (LWR) systems. These studies include, inter alia, neutronic and thermal hydraulic analyses of selected LWR systems. Studies that were conducted by the school include amongst others, elements of the safety analysis of the European Pressurized Reactor (EPR) and of the Vodo-Vodyanoi Energetichesky Reaktor or Water-Water Energetic Reactor (VVER). Furthermore, the research team is actively engaged in benchmark activities, such as that of modelling the MIT BEAVRS benchmark.

The study carried out in this dissertation focuses on testing the HEADE collision probability code for modelling PWR's, with specific focus on the MIT BEAVRS benchmark.

HEADE, an in-house lattice code developed and maintained by Necsa's Radiation and Reactor Theory (RRT) group as part of the OSCAR-4 system, is currently used as a cross-section generation module for SAFARI-1 research reactor assemblies (fuel and non-fuel assemblies) as well as at other international research reactors such as HFR and HOR in the Netherlands and the McMaster Research Reactor in Canada.

HEADE has been chosen amongst many other codes as it has been developed in South Africa. The code has an extensive and proven record in modelling research reactor plate type fuel assemblies; however its applicability to PWR pin-type assemblies is limited. Thus

the aim of the study is to test the code's (HEADE) capabilities in modelling modern pin-type assemblies. The MIT BEAVRS benchmark specification will be used in this case.

In addition, the results of this study will provide valuable information and a possible platform for the use of the HEADE code, as part of the OSCAR-4 system as a cross-section generation module for neutronic calculations for the envisaged South Africa nuclear power plant fleet. Furthermore, the study provides skills training for students in neutronic code applications.

1.3 Problem Statement

Necsa has developed a core calculation code, OSCAR-4, which is currently used at the SAFARI-1 research reactor. OSCAR-4 has HEADE as one of its constituent sub-codes. HEADE is used as a cross-section generation module for fuel and non-fuel assemblies. The applicability of HEADE to model PWR pin-type assemblies has not been tested. Therefore this study seeks to address the following question:

Does the HEADE collision probability code have the capabilities for modelling modern pin-type assemblies?

A selection of fuel assemblies from the MIT BEAVRS benchmark will be used in judging the capability of the HEADE code. HEADE will be compared with the Serpent Monte Carlo code models.

1.4 Objectives

The objectives of the study are the following:

- a. Compare HEADE and Serpent burn-up results;
- b. Determine the effects of a spacer grid on the multiplication constant of a fuel assembly;
- c. Determine the effects of changing fuel enrichment in a fuel assembly; and
- d. Determine the effects of adding control rods, burnable poison and an instrumentation tube to a fuel assembly.

1.5 Organization of Dissertation

This dissertation is presented in six (6) chapters. The current chapter, which is Chapter 1 of this dissertation, is an introductory chapter which provides a brief background and overview of the study documented in this dissertation. The sections that follow the brief background describe the motivation for the study, the overall objective of the study presented in this document as well as the organization of this document. Chapter 2 provides a brief description of nuclear reactors (MIT BEAVRS benchmark in particular) and some literature of similar work that has been done by other researchers that is relevant to this study. A brief description of the HEADE collision probability code as well as the Serpent Monte Carlo code is also given in the chapter. Chapter 3 covers the theory on the overall reactor physics concepts relevant to this study. In Chapter 4, the methods that were followed in carrying out the investigation are provided. Chapter 5 presents the results of this study as well as a discussion of the results obtained. This document is concluded, in Chapter 6, with the assessment of the progress made towards the initial goal set out by the research leading to conclusions and recommendations.

CHAPTER 2 LITERATURE STUDY

2.1 The Pressurized Water Reactor

Electricity is produced from, amongst others, many different types of nuclear power reactors operated around the world. These types of power reactors are described in more detail in many texts, such as (Lewis, 2008); (Lamarsh & Baratta, 2012) and (Stacey, 2007). Furthermore, new nuclear power reactors are being constructed around the world; the majority are PWRs. A PWR as shown in Figure 2-1 is basically a two-loop system where the coolant in the primary loop (in red/yellow) is heated up in the reactor core and the energy gained is transferred to the coolant in the secondary loop (in blue) using a heat exchanger. The turbine is driven by the steam in the secondary system and electricity is produced. Figure 2-1 illustrates the PWR two-loop steam cycle. It should be noted that there can be more than one leg in both the primary and secondary loops.

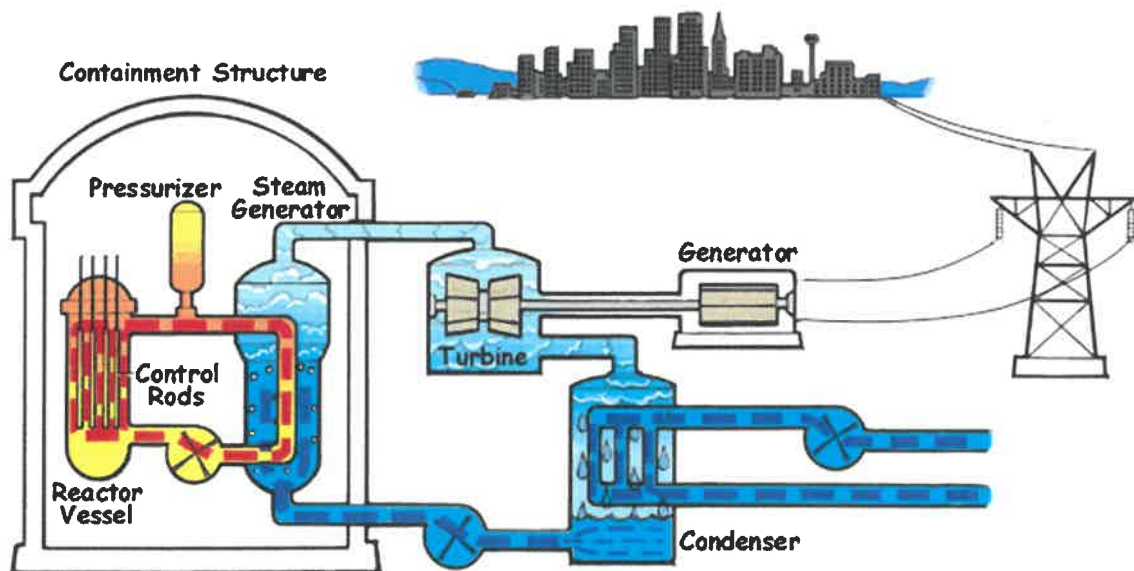


Figure 2-1: PWR two-coolant steam cycle (USNRC, 2016)

2.1.1 Reactor core

In a nuclear reactor, the reactor core is located in a reactor vessel. Pressurized light water which acts both as moderator and coolant, flows through the reactor core. A schematic diagram of a typical PWR core is shown in Figure 2-2.

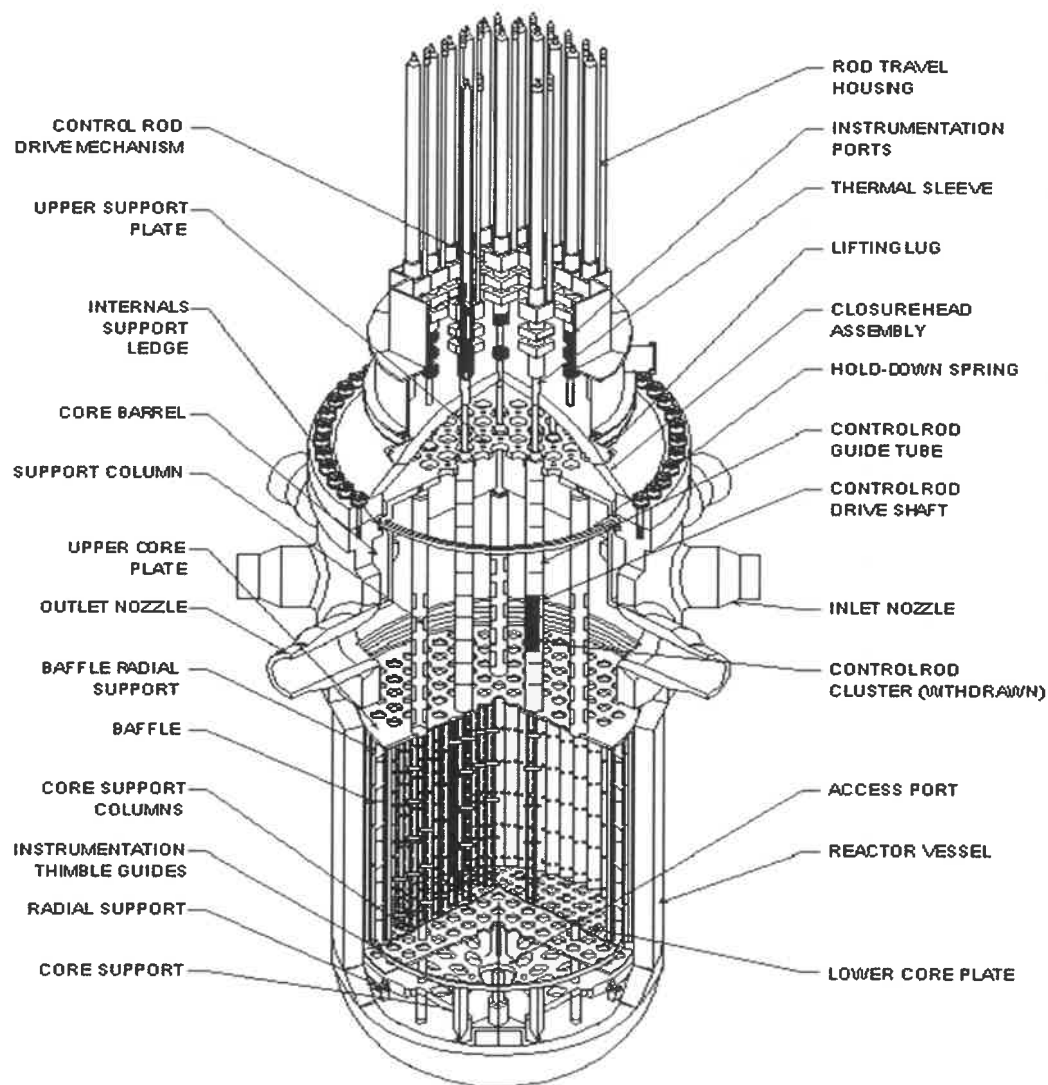


Figure 2-2: Schematic diagram of a typical PWR core (EIA, 2015)

The basic component of the core is the cylindrical fuel pellet which is composed of slightly enriched uranium dioxide (UO_2) powder that is compacted by cold pressing and then sintered to attain the required density. Uranium dioxide pellets are inserted into a Zircaloy-4 tube, and each end of the tube is sealed by welding on an end plug

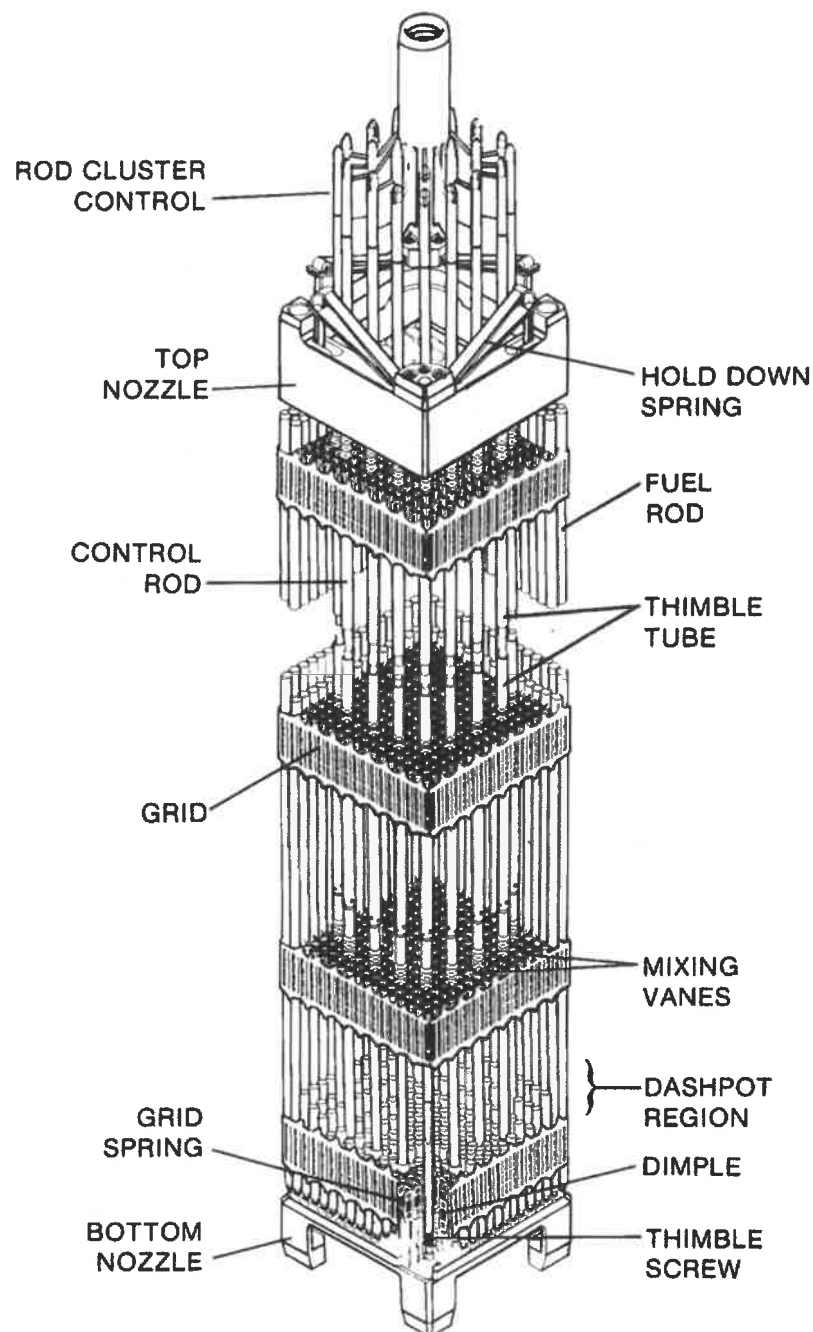


Figure 2-3: Fuel assembly for a pressurized water reactor (Westinghouse, 1984)

to form a fuel rod. The basic structure of the Pressurized Water Reactor (PWR) core is the fuel assembly which consists of an array of Zircaloy-clad UO_2 fuel rods as shown in Figure 2-3. It is approximately 20 cm x 20 cm x 4 m high. A typical fuel assembly may consist of a 17 x 17 array of fuel rods of about 1 cm diameter and a typical PWR core is constituted of about 190 to 240 fuel assemblies containing 90 000 to 125 000 kg of UO_2 (Stacey, 2007).

2.1.2 Spacer grid

The radial spacing of fuel assemblies is maintained by the spacer grid structures located at specified intervals along the entire length of the assembly. Nine spacer grids are typically applied to a 17 x 17 assembly. The rods are kept in position by the spacer grids, using a combination of dimples and springs. The design of these spacer grids allows axial and radial thermal expansion of the fuel rods in order to minimize their deformation. Some spacer grids contain mixing vanes to promote coolant flow. The spacer grids are made of Zircaloy material. Figure 2-4 shows a typical spacer grid.

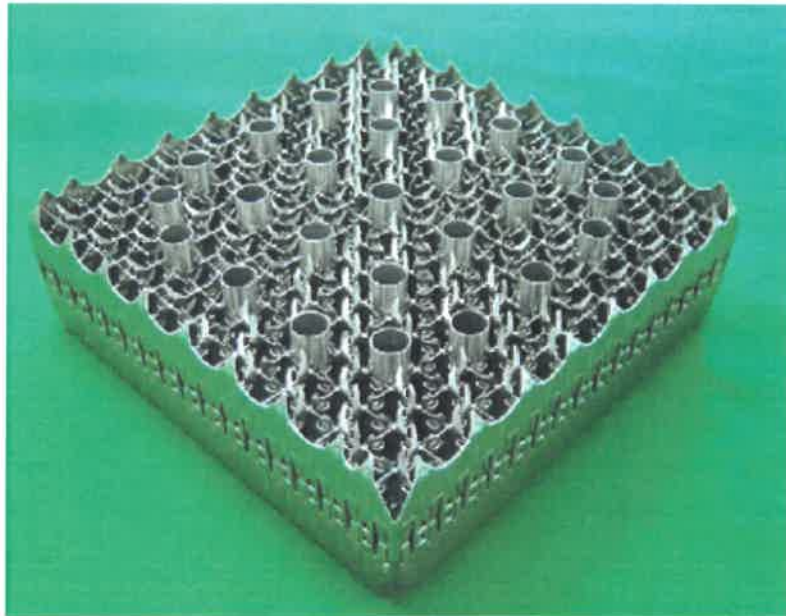


Figure 2-4: PWR spacer grid (*Buongiorno, 2010*)

2.2 BEAVRS Benchmark Overview

This section gives an overview of the BEAVRS benchmark with specific focus on the fuel assemblies selected for this study. The BEAVRS benchmark provides very detailed design data for the first two cycles of a real PWR, as well as corresponding measurement data. Such publicly available core benchmark data allows for code validation without the need for access to proprietary information. This makes BEAVRS an ideal choice for validation and comparison between different codes.

BEAVRS is a multi-cycle full-core Pressurized Water Reactor (PWR) depletion benchmark. This benchmark is based on two operational cycles of a commercial nuclear power plant that provides a detailed description of fuel assemblies, burnable absorbers, in-core fission detectors, core loading and reloading patterns. This benchmark has been chosen as it

enables analysts to develop detailed reactor core models that can be used for testing and validation of coupled neutron transport, thermal-hydraulics, and fuel isotopic depletion. The BEAVRS benchmark also provides measured reactor data for hot zero power (HZP) physics tests, boron let-down curves, and three-dimensional in-core flux maps from fifty-eight instrumented assemblies as stated in (Forget, et al., 2014).

Figure 2-5 represents the initial cycle 1 fuel assembly loading pattern of the BEAVRS benchmark core, including the distribution of enrichment as well as burnable absorber locations. Each of the fuel assemblies in the core is made up of a 17 x 17 array of pins. A representation of a standard fuel assembly is shown in Figure 2-6. In this study, the focus is on models of selected fuel assemblies of the BEAVRS benchmark. The selected fuel assemblies are introduced in the following paragraph.

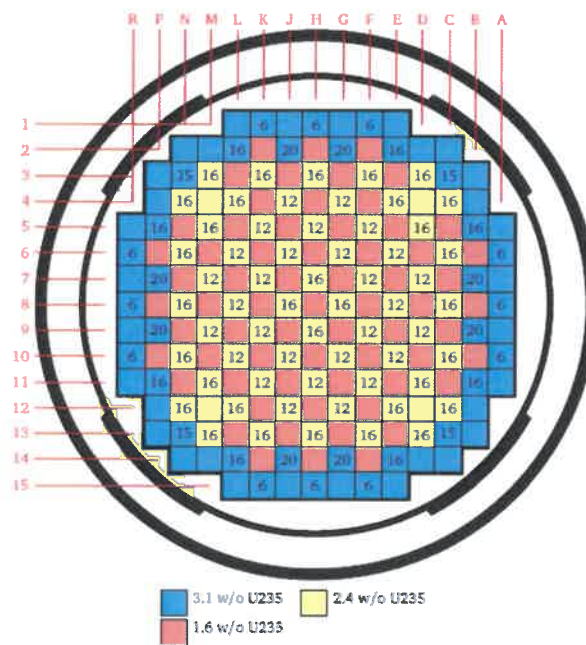


Figure 2-5: Layout of fuel assemblies showing enrichment loading pattern and burnable absorber positions in cycle 1 (Horelik & Herman, 2013)

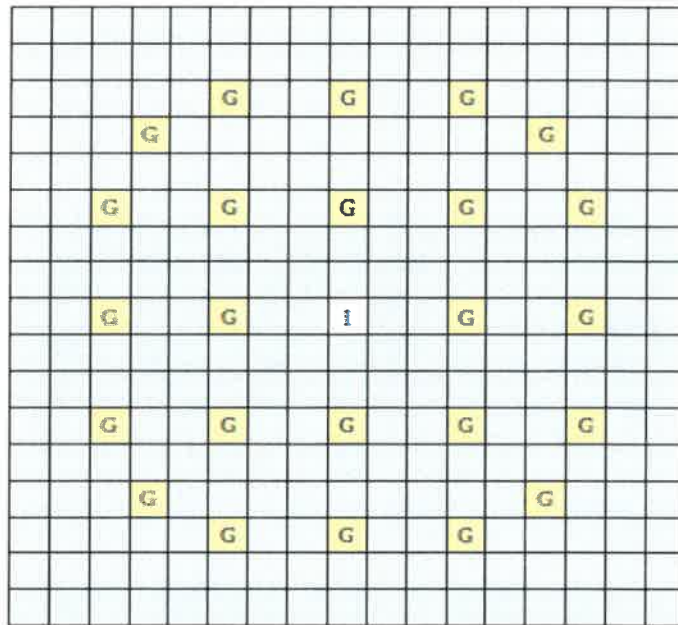


Figure 2-6: Fuel assembly guide tube locations. Blank denotes fuel rods, G denotes a guide tube location, and I denotes a guide tube position that might contain an instrument tube (Horelik & Herman, 2013)

2.3 Description of the Fuel Assemblies Selected from the BEAVRS Benchmark

In this section, the 6 BEAVRS benchmark fuel assemblies that have been selected for this study are described. The fuel assemblies that have been selected are the following: J9; M12; R9; K8; J7 and K9 (see Figure 2-5). These fuel assemblies are comprised of the following:

1. Fuel assemblies J9, M12 and R9 consist of 264 fuel rods with a 1.6 %, 2.4 % and 3.1 % ^{235}U enrichment respectively. They all have 24 empty guide tubes and 1 empty instrument tube in the centre. These are arranged as in Figure 2-6.
2. Fuel assembly K8 consists of 264 fuel rods with a 1.6 % ^{235}U enrichment, 24 control rods in the empty guide tube positions and 1 empty instrument tube in the centre. These are arranged as in Figure 2-6 except that the control rods are present in the 24 guide tube places.
3. Fuel assembly J7 consists of 264 fuel rods with a 1.6 % ^{235}U enrichment, 24 empty guide tubes and 1 instrument tube in the centre. These are arranged as in Figure 2-6 as well.

4. Fuel assembly K9 consists of 264 fuel rods with a 1.6 % ^{235}U enrichment, 12 empty guide tubes and 1 empty instrument tube in the centre and 12 burnable absorber rods. These are arranged as in Figure 2-7.

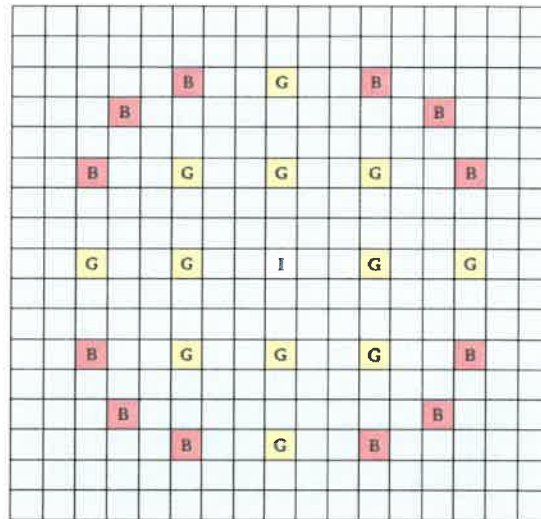


Figure 2-7: The 12BA burnable absorber configuration. Blank denotes fuel rods, G denotes a guide tube location, B denotes a burnable absorber rod, and I denotes a guide tube that might contain an instrument tube (Horelik & Herman, 2013)

The geometry of the fuel rod, empty guide tube, control rod pin, instrument tube pin, and burnable poison pin are as shown in Figure 2-8, 2-9, 2-10 2-11 and 2-12 respectively.

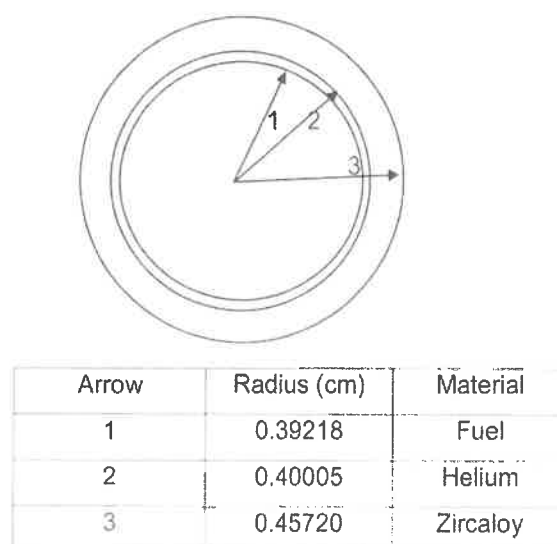
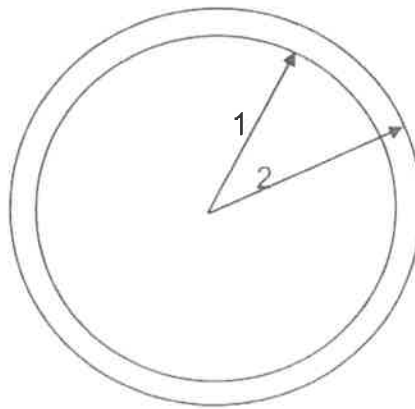
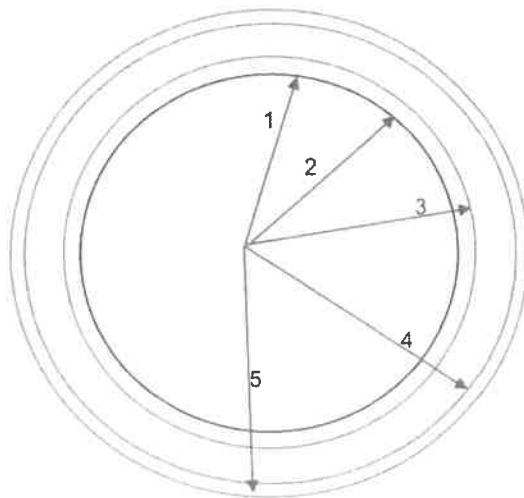


Figure 2-8: Fuel pin diagram and the radii



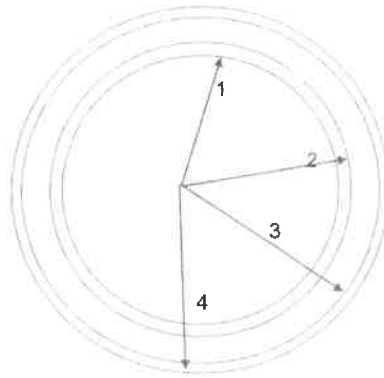
Arrow	Radius (cm)	Material
1	0.56134	Water
2	0.60198	Zircaloy

Figure 2-9: Empty guide tube diagram and the radii



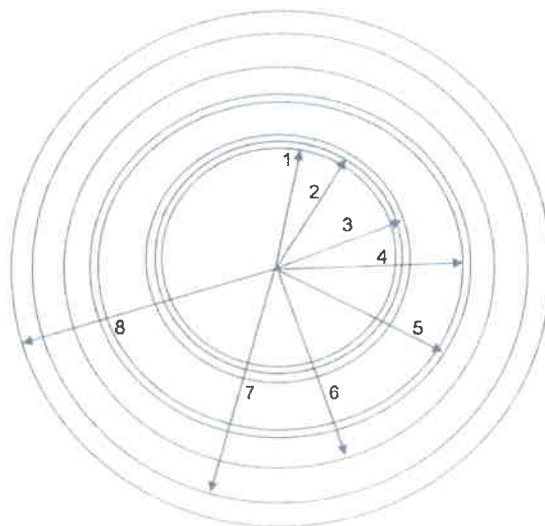
Arrow	Radius (cm)	Material
1	0.43310	Ag-In-Cd
2	0.43688	Air
3	0.48387	SS304
4	0.56134	Water
5	0.60198	Zircaloy

Figure 2-10: Control rod pin geometry



Arrow	Radius (cm)	Material
1	0.43688	Air
2	0.48387	Zircaloy
3	0.56134	Water
4	0.60198	Zircaloy

Figure 2-11: Instrument tube pin geometry



Arrow	Radius (cm)	Material
1	0.21400	Air
2	0.23051	SS304
3	0.24130	Air
4	0.42672	Borosilicate Glass
5	0.43688	Air
6	0.48387	SS304
7	0.56134	Water
8	0.60198	Zircaloy

Figure 2-12: Burnable poison above dashpot

Table 2-1 shows some of the useful fuel assembly parameters as given in the BEAVRS handbook.

Table 2-1: Fuel assembly parameters as given in the BEAVRS handbook

Core Power	3411 MWth
Active Fuel Length	365.76 cm
Operating Pressure	2250 psia
Pitch	12.5984 mm
Fuel Height	388.112 cm
Cladding	Zircaloy-4
Boron Concentration	975 ppm

2.4 Review of Studies Involving the MIT BEAVRS Benchmark

Findings/conclusions of some selected papers based on the performance of various neutronic codes of the BEAVRS benchmark are discussed in this section. The conclusions of these studies will be very useful in interpreting and understanding the results of the current study.

A. Solution of the BEAVRS benchmark using CASMO-5/SIMULATE-5 code sequence (Bykov V., Vasiliev A., Ferroukhi H., and Pautz A.).

The work of (Bykov, et al., 2016) focused on the critical boron concentration (CBC) and the in-core detector comparisons. The best results were obtained with SIM-3. SIM-5 systematically underestimated critical boron by approximately 50 ppm compared to SIM-3. The removal of the thermo-hydraulics (TH) module reduced that difference, while the use of a SIM-5 macroscopic depletion model further increased that difference.

This study demonstrates that the BEAVRS benchmark is very useful as it could be used for code validation without access to proprietary information being needed.

B. Analysis of the MIT BEAVRS benchmark using the DRAGON-5/PARCS code sequence (Taforeau J. and Salino V.).

In this study, the DRAGON-5 lattice code was used for the production of a parameterized macroscopic cross-section library at the assembly level. A CASMO-5 calculation was also performed for comparison with cross-sections by DRAGON-5.

The cross sections produced by the DRAGON-5 lattice code are compared to the deterministic reference calculation CASMO-5 and a Monte Carlo McCARD was published. The reactivity of fuel assemblies at hot zero power (HZP) was benchmark compared for the different codes used. This part of the study contributes to the methodology adopted in the current study.

Comparison with both benchmark data and deterministic reference codes showed consistency of the DRAGON-5/PARCS method for the characterization of a PWR core reactor. There was a good agreement between the control rod worth and isothermal coefficient calculation (Taforeau & Salino, 2016).

C. Analysis of BEAVRS two-cycle benchmark using RMC based on full core detailed model (Wang K, et al., 2017).

In this study the radial detectors' response in the instrument rod located in the centre of some assemblies were calculated and compared with the benchmark results. The results of RMC agree well with the given data of a BEAVRS benchmark and also agree well with existing MC21 code results. The manner in which the two are compared contributes to the methodology that is adopted in the current study.

2.5 Computer Codes Used in this Study

The two codes used in this study were the HEADE probability code and the Serpent Monte Carlo code. These codes are briefly introduced in this section.

2.5.1 HEADE collision probability code

The HEADE code is part of the OSCAR-4 calculation system (Prinsloo, 2009). The OSCAR-4 code is a reactor calculation system, with specific focus on research reactor calculation support, used at the SAFARI-1 Research Reactor and other international research reactors, viz.: HFR, and HOR (in the Netherlands) and the MacMaster Reactor (in Canada). There is a possibility that OSCAR-4 and/or later versions, can be used to model the PWR reactors that are envisioned for the South African nuclear new build. Neutronics models will therefore need to be built, and a good starting point would be the lattice models of the fuel assemblies using HEADE.

The OSCAR-4 system consists of three modules namely: CROGEN, CROLIN and CORANA. CROGEN contains codes used for creating few-group cross-section tables for various assembly types and configurations. One of these codes is HEADE. CROLIN parameterizes the cross-section tables, which are produced in CROGEN, and combines these parameterized cross-sections for different assemblies into one cross-section library for the reactor. CORANA is the diffusion based core simulator suite (Bokov & Botes, 2009).

HEADE stands for "HEterogeneous Assembly DEpletion" code. It is a two-dimensional code that is used in the generation of few-group homogenized cross-sections. HEADE is a collision probability transport solver based on Equation 3.9 in this dissertation. It utilizes a response matrix formalism to solve a 2-D fine-group transport problem for a given assembly type. HEADE can also perform fuel assembly depletion calculations. The code incorporates all the functions required for generating few-group homogenized assembly cross-sections, flux/power form functions and interface flux discontinuity factors as functions of exposure, water density, water temperature, fuel temperature, control rod status, etc. (Müller, et al., 1-6 05 1994). The specification as stated in Table 2-1 are used as input in the HEADE input file. The HEADE code allows one to vary parameters such as fuel temperature/density, moderator temperature/density, boron concentration, etc. within a single run, and writes the discreet set of homogenized cross-section data, generated by utilizing the transport solution as a weighting function for both spatial homogenization and energy condensation. This results in the creation of the PRT file and the HED file. The HED file is the specific format in which the homogenized cross-sections are passed to the next step in the calculation path. The PRT file is the print out file for the run, which contains a user interpretable summary of calculational results including fine group flux profiles, infinite multiplication factors and broad group cross-sections (Prinsloo, 2009).

The specific solution algorithm in HEADE (low order response matrix scheme) does however make certain assumptions in solving the transport problem. In particular, very sharp flux gradients and strong anisotropic behaviour may diminish the accuracy of the HEADE solution.

The HEADE collision probability lattice code uses a response matrix solution scheme. The coupling between response matrices is done via a low-order cosine current approximation

for the angular flux on interfaces, while the solution within each cell is performed with collision probabilities.

HEADE uses a 172-group, Christmas structure WIMS-E format fine-group cross-section library, largely based on cross-sections from JEFF 2.2 (Anon., March 1996). This library contains all the required parameters for multi-group lattice calculations in terms of fine-group cross-sections and resonance parameters, and was generated with a typical LWR slowing down spectrum.

2.5.2 Serpent Monte Carlo code

The Serpent code is a high-fidelity, highly accurate Monte Carlo based lattice code written in standard ANSI-C language. The code is mainly developed in the Linux operating system, but it has also been compiled and tested in MAC OS X and some UNIX machines. The Monte Carlo method is a computing-intensive calculation technique and raw computing power has a direct impact on the overall calculation time. Serpent is a continuous energy Monte Carlo reactor physics burn-up calculation code (Leppänen, 2015).

It is specially optimized for the homogenized group constants generation. In addition, Serpent has built-in capabilities to perform fuel depletion calculations without relying on external codes or wrapper scripts. It also has an advantage of automatically performing the depletion sequence and requested restart cases needed in a typical process of a few-group constants generation (Luszczek, 2015).

In developing the model, the geometry and material composition must be carefully defined, together with the run parameters such as the total number of cycles. The code then calculates the multiplication factor. Tallies and group constants can also be generated.

The Serpent models used in this study were developed for comparison with the HEADE models. Comparison of the results of the two codes, HEADE and Serpent, is dealt with in Chapter 5 of this dissertation.

CHAPTER 3 THEORY

In this chapter, the theory relevant to the investigation discussed in this dissertation is briefly presented.

3.1 Neutron Reactions

There are various neutron reactions that take place in a nuclear reactor. The types and rates of neutron reactions depend on the neutron energy and the nuclide it collides with. The important reactions are explained below.

3.1.1 Scattering of neutrons

Scattering is a reaction in which the emitted particle is of the same kind as the incident one. Two kinds of scattering, elastic scattering and inelastic scattering have been identified. In elastic scattering kinetic energy and momentum of the neutron and the isotope are conserved and the nuclear energy state of the isotope does not change. If the neutron energies before and after the collision are E and E' , the relationship between the incident and the final energies of the neutron in the lab system and the scattering angle in the centre-of-mass system is given by:

$$\frac{E'}{E} = \frac{(1+\alpha) + (1-\alpha)\cos\theta_c}{2} \quad 3.1$$

where $\alpha = (A - 1)^2 / (A + 1)^2$, A is the atomic number of the scattering isotope and θ_c is the scattering angle in the centre-of-mass coordinate system (Stacey, 2007).

In the case of inelastic scattering, a collided nucleus is excited and the energy of the scattered neutron together with the energy of the nucleus due to recoil decreases by the amount of the excitation energy transferred to the nucleus. In order for excitation to occur, the energy of the reacting neutron and scatter must be equal or greater than the excitation energy. In general, the heavier the nuclide, the more densely the energy levels are distributed, and thus heavier nuclides have a larger cross-section for inelastic scattering (Sekimoto, 2007).

3.1.2 Nuclear fission

Nuclear fission is observed in heavy nuclei. It is only ^{235}U amongst the naturally-occurring nuclides that can fission by thermal neutrons. If the energy of the neutrons is increased, ^{238}U and ^{232}Th can fission. Nuclear fission by a thermal neutron is called thermal fission and that by a fast neutron is called fast fission. When nuclear fission takes place, the nucleus splits into two or more fission fragments. When a thermal neutron is incident on ^{235}U , an average of 2.4 neutrons is generated. This enables a chain reaction (Sekimoto, 2007).

3.2 Nuclear Fission Chain Reaction

Nuclear energy is released by way of a fission chain reaction in the fuel in the reactor vessel. In that process, neutrons emitted by fission nuclei induce fission in other fissile nuclei; the neutrons from these fissions induce fissions in still other fissile nuclei and so on. Neutrons in a nuclear reactor behave as shown in Figure 3-1.

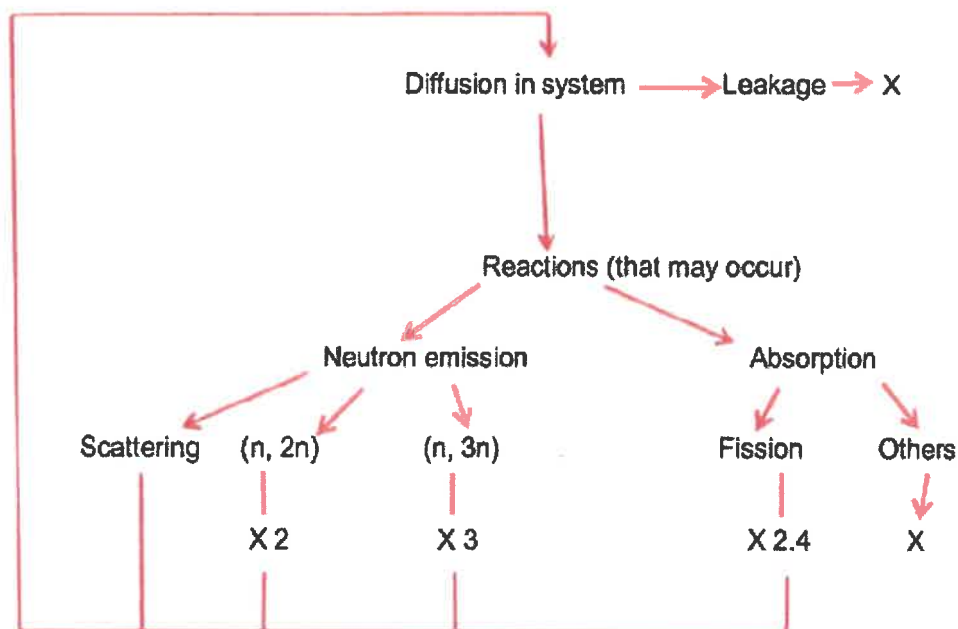


Figure 3-1: Neutron behaviour in a nuclear reactor

Such a chain reaction can be described in terms of the multiplication factor, which is denoted by the letter k (Lamarsh & Baratta, 2012). It is expressed as follows:

$$k = \frac{\text{Number of neutrons in one generation}}{\text{Number of neutrons in the preceding generation}} \quad . \quad 3.2$$

If k is greater than 1, the number of fissions increases from generation to generation and the system is said to be supercritical. If k is less than 1, the number of fissions decreases from generation to generation and the system is said to be subcritical. When k equals 1, the chain reaction proceeds at a constant rate and the system is said to be critical (Lamarsh & Baratta, 2012).

It is known that thermal reactors contain fuel, coolant, various structural materials and a moderator to slow down the fission neutrons to thermal energies. In a critical reactor there is a balance between the number of neutrons produced in fission and the number lost, either by absorption in the reactor or by leaking from its surface (Todreas & Kazimi, 1990). When a nuclear reactor is assumed to be infinitely large and there is no neutron leakage, the multiplication factor is called the infinite neutron multiplication factor and is denoted by k_{inf} .

3.3 Neutron Flux

Considering a reaction of a neutron and a nucleus, it is convenient to define the neutron flux as the product of the neutron number density n and velocity v :

$$\phi(r, E, t) = vn(r, E, t) \quad . \quad 3.3$$

where, r is the physical position at which n is defined, E is the energy of the neutron, t is the time and v is the velocity of the neutron.

3.4 Reaction Rate and Cross-Section

The reaction rate R can be expressed using the neutron flux as follows:

$$R(r, t) = \int_0^{\infty} N\sigma(E)\phi(r, E, t)dE \quad 3.4$$

where, N is the number density of the target nucleus and σ is a proportionality constant called the microscopic cross-section. The microscopic cross-section is a very small value and it is normally measured in the units of 1 barn = 10^{-24} cm². σ appears as a product with N as shown, $\Sigma = \sigma N$. Σ is called the macroscopic cross-section and has the dimension of cm⁻¹.

3.5 Neutron Transport Equation

The neutron transport equation is the central equation used in transport theory. The standard form of the neutron transport equation is given by:

$$\begin{aligned} \frac{1}{v} \frac{\partial \psi}{\partial t}(\mathbf{r}, \boldsymbol{\Omega}, t) + \boldsymbol{\Omega} \cdot \nabla \psi(\mathbf{r}, \boldsymbol{\Omega}, t) + \Sigma_t(\mathbf{r}) \psi(\mathbf{r}, \boldsymbol{\Omega}, t) \\ = \int_{-1}^1 d\mu_0 \Sigma_s(\mathbf{r}, \mu_0) \psi(\mathbf{r}, \boldsymbol{\Omega}', t) \\ + \frac{1}{4\pi} \int_0^{4\pi} d\boldsymbol{\Omega}' v \Sigma_f(\mathbf{r}) \psi(\mathbf{r}, \boldsymbol{\Omega}', t) + S_{ex}(\mathbf{r}, \boldsymbol{\Omega}) \equiv S(\mathbf{r}, \boldsymbol{\Omega}) \end{aligned} \quad 3.5$$

where $\mathbf{r}$ is the position of neutron motion in space, $\boldsymbol{\Omega}$ is the direction of neutron motion after scattering, t is the time, v is the neutron speed after scattering, Σ_t is the macroscopic total cross-section, Σ_s is the macroscopic scattering cross-section, $\boldsymbol{\Omega}'$ is the direction from which the neutron is being scattered, S is the source of neutrons and $\psi(\mathbf{r}, \boldsymbol{\Omega}, t) \equiv vN(\mathbf{r}, \boldsymbol{\Omega}, t)$ is a quantity known as angular neutron flux.

Boundary conditions for Equation 3.5 are generally specified by the physical situation. For left boundary at $\mathbf{r}_L$ with inward normal vector $\mathbf{n}$, such that $\mathbf{n} \cdot \boldsymbol{\Omega} > 0$ indicates inward, one of the following boundary conditions is usually appropriate:

Vacuum:	$\psi(\mathbf{r}_L, \boldsymbol{\Omega}) = 0, \quad \mathbf{n} \cdot \boldsymbol{\Omega} > 0$	
Incident flux known:	$\psi(\mathbf{r}_L, \boldsymbol{\Omega}) = \psi_{in}(\mathbf{r}_L, \boldsymbol{\Omega}), \quad \mathbf{n} \cdot \boldsymbol{\Omega} > 0$	
Reflection:	$\psi(\mathbf{r}_L, \boldsymbol{\Omega}) = \int_0^{4\pi} \alpha(\boldsymbol{\Omega}' \rightarrow \boldsymbol{\Omega}) \psi(\mathbf{r}_L, \boldsymbol{\Omega}') d\boldsymbol{\Omega}'$	3.6

where α is a reflection or albedo function (Stacey, 2007).

The steady-state form of the transport equation is written as:

$$\frac{d}{dR} \psi(\mathbf{r}, \boldsymbol{\Omega}) d\mathbf{r} d\boldsymbol{\Omega} + \Sigma_t(\mathbf{r}) \psi(\mathbf{r}, \boldsymbol{\Omega}) d\mathbf{r} d\boldsymbol{\Omega} = S(\mathbf{r}, \boldsymbol{\Omega}) d\mathbf{r} d\boldsymbol{\Omega} \quad 3.7$$

where dR is the differential length along the direction $\boldsymbol{\Omega}$. Integrating Equation 3.7 along the direction $\boldsymbol{\Omega}$ from $\mathbf{r}_0$ to $\mathbf{r}$ gives:

$$\psi(\mathbf{r}, \boldsymbol{\Omega}) d\mathbf{r} = e^{-\alpha(\mathbf{r}_0, \mathbf{r})} \psi(\mathbf{r}_0, \boldsymbol{\Omega}) d\mathbf{r}_0 + \int_{\mathbf{r}_0}^{\mathbf{r}} e^{-\alpha(\mathbf{r}', \mathbf{r})} S(\mathbf{r}', \boldsymbol{\Omega}) d\mathbf{r}' \quad 3.8$$

where $\alpha(\mathbf{r}', \mathbf{r})$ is the optical path length along the direction $\boldsymbol{\Omega}$ between $\mathbf{r}'$ and $\mathbf{r}$, (Stacey, 2007):

$$\alpha(\mathbf{r}', \mathbf{r}) \equiv \int_{\mathbf{r}'}^{\mathbf{r}} \Sigma_t(R) dR$$

Using this integral transport equation, the collision probability method can be formulated. In HEADE, this formulation is based on the following equation as derived by Stacey.

$$\phi_i = \sum_j T^{j \rightarrow i} [(\Sigma_{sj} + v\Sigma_{fj})\phi_j + S_{0j}]. \quad 3.9$$

Here, the problem of interest is partitioned into discrete volumes, V_i . Within each volume, uniform average cross-sections are assumed, such as Σ_{si} which is shown in Equation 3.9 as Σ_{sj} . A flat flux, ϕ_i , is assumed in each volume i . $T^{j \rightarrow i}$ is the first flight transmission probability between cell i and j .

3.6 Stochastic Methods Used to Solve Neutron Transport

An alternate to solving the transport equation as discussed in the sections above, is to solve the neutron transport using stochastic methods. These are the so-called Monte Carlo methods.

Monte Carlo methods have no need for a direct solution of the neutron transport equation as they do not discretize it the same way deterministic codes do. Instead they are able to explicitly simulate the interactions between neutrons and isotopes. By tracing the path of an individual neutron as it traverses matter and considering the various processes that may determine its history, a Monte Carlo calculation simulates the stochastic nature of neutron transport through matter. A brief description of the process is given below.

The starting point is to define the source of neutrons in a nuclear reactor. The fission source has a distribution in space, a distribution in energy given by the fission spectrum, and a distribution in direction that is isotropic. Each of these distributions may be characterized by a probability distribution function (pdf) and a cumulative distribution function (cdf) (Stacey, 2007).

Generating a random number and selecting from the cdf for the spatial fission distribution shall define a location in space for the source particle. Generating another random number and selecting from the cdf for the fission spectrum shall determine the energy of the source particle. When generating third and fourth random numbers and selecting from the cdf's for the two independent angular variables will define the direction of the source neutron. The fission source is therefore defined using a random process. The history of each source neutron is then tracked.

Once launched, the source neutron will travel in a straight line until it collides. The probability that a neutron will collide at a distance s along the path of flight is given by:

$$T(s) = \Sigma_t \exp\left[-\int_0^s \Sigma_t(s') ds'\right] \quad 3.10$$

which is the pdf for the collision distance s . Generating a random number λ and selecting s from the cdf

$$-\ln\lambda = \int_0^s \Sigma_t(s') ds' \quad 3.11$$

will locate the position of the first collision (Stacey, 2007).

Having determined that a collision occurred at a distance s_n into region n on the original path of flight, it is necessary to determine the type of nuclide and the type of reaction that are involved. The probability for a reaction of type x with a nuclide of species i is given by:

$$p_{ix} = \frac{N_i \sigma_{ix}}{\sum_{i,x} N_i \sigma_{ix}} \quad 3.12$$

where N_i is the number density of nuclide i in region n , σ_{ix} is the microscopic cross-section for reaction x for nuclide i at the energy of the neutron. Constructing a pdf and a cdf, generating a random number η , and selecting the nuclide and reaction type by equating η and the cdf, the nuclide and reaction type can be determined (Stacey, 2007).

For the absorption type of reaction, the neutron history is terminated, the energy and location of the absorbed neutron are recorded, and another history is started. If the reaction type is elastic scattering, the history of the neutron continues. Another random number is generated and equated to the cdf for the cosine of the scattering angle in the centre-of-mass (CM) to obtain μ_{cm} and by transformation to obtain the scattering angle in the lab. Considering energies above thermal, the energy of the scattered neutron is uniquely correlated to μ_{cm} from the scattering kinematics:

$$E' = \frac{E'(A^2 + 2A\mu_{cm} + 1)}{(A+1)^2} \quad 3.13$$

If E' is known, the cosine of the scattering angle in the lab can be determined from:

$$\mu = \cos\theta = \frac{1}{2}(A+1)\sqrt{\frac{E}{E'}} + \frac{1}{2}(A-1)\sqrt{\frac{E}{E'}} \quad 3.14$$

Generating another random number and equating it to the cdf for the azimuthal angle ϕ , the direction of the scattered neutron can be determined. The scattered neutron is treated as described above for a fission source neutron, and the calculation is repeated until the neutron either leaks from the system or is absorbed (Stacey, 2007).

The process is repeated for all the neutrons in a given generation. When all the histories have been processed, the multiplication factor is obtained as the ratio of the number of fission neutrons produced in the generation to the initial number of source neutrons in the generation.

The process is then repeated for the next generation, where the fission of the previous generation is used as the source neutrons for the next generation, with an appropriate normalization to keep the number of source neutrons constant for each generation. After calculating the multiplication factor for a number of generations, the statistical average can be calculated. It is noted that the statistical average can only be counted at the generation when the source distribution is considered to be sufficiently spread out on all fission cells.

The flux can also be obtained by evaluating the neutron presence in the geometric cells of the problem. Two possible methods are the collision rate estimator and the track length estimator.

One of the remarkable features of the Monte Carlo method when handling neutron transport is that the quantities it actually solves for may be very different from each other. Thus, it makes codes such as Serpent, which is based on the Monte-Carlo method, a very flexible and versatile tool (Luszczek, 2015). Monte Carlo calculations only provide information for the specified parameters being tallied, not necessarily the quantities present in the transport equation.

3.7 Reactor Calculation Strategy

There are many types of calculations that must be carried out in the reactor core and related structures, such as criticality and shielding. In criticality calculations, one is primarily concerned with calculating the neutron flux, since the other related quantities such as the reaction rates and power profiles can be calculated from the neutron fluxes and the isotopic cross-sections. These calculations are carried out by solving some form of neutron transport equation.

However, when using deterministic methods to solve the neutron transport equation, the solution becomes intractable if the entire core is solved in one attempt, even numerically. This is because the reactor core is highly heterogeneous. It is therefore the practice to

break up the calculation into a series of calculations. The steps in a typical analysis would comprise of cell calculations, lattice calculations and core calculations. Cell calculations are models of the fuel pin and its immediate surroundings, and are done to take into account the effect that the resonance absorbers have on the flux profiles. In lattice calculations, two-dimensional models of fuel assemblies are normally carried out. The spatial and angular nature of the flux is maintained together with the dependence on energy. However, some homogeneity in the energy variable is obtained by splitting the energy range into a number of energy groups. The typical number of energy groups is above 200 for thermal reactors (Leppänen, et al., 2016) and (C'alic', et al., 2016).

In core calculations, the entire core or a symmetry section of the core is considered and the flux and the multiplication constant are calculated. In this part of the calculation, the high dependence on energy is reduced typically to two groups for light water reactors. If one uses diffusion theory, then the angular dependence of the neutron flux is also significantly simplified.

The key to separating the reactor analysis into a number of calculation steps is that the local reaction rate is preserved at each stage. By using this method a tractable solution to the problem is achieved.

In the OSCAR-4 code suite, the cell calculations are carried out using lattice calculations in the HEADE code and the core calculation is carried out by using the code MGRAC (Müller, et al., 1-6 05 1994).

The neutron diffusion equation is also used for some applications, in which a form of Fick's law is used in the neutron transport equation. The diffusion equation is mainly used for all the reactor core calculations in which the multiplication factor and neutron fluxes are evaluated. Neutron transport is applied at lattice/cell level to account/capture as much details as possible (geometric, composition, etc.). Unlike the diffusion equation, the transport equation is computationally expensive (or impossible in most cases) when applied to the whole core calculation hence the diffusion approximation is applied. However, due to the complicated nature of these lattice/cell calculations, 2-D calculations are normally carried out, i.e. slices of the fuel assembly are considered (Sekimoto, 2007).

3.8 Group Constants

It has been mentioned that the energies of all the neutrons are divided into a number of energy groups to simplify the energy description. The neutrons within each group are then lumped together and their scattering, absorption, and other interactions are described in terms of suitably averaged parameters which are collectively known as group constants (Lamarsh & Baratta, 2012).

When conducting lattice and core calculations, group constants are required. For the lattice calculations, these are calculated in the cell calculation as discussed in the section on reactor calculation strategy. The spatial detail of the cell is considered in calculating the self-shielding effect of the resonance absorbers.

For the core calculations, the group constants are calculated in the lattice calculations. The normal practice would be to consider a slice of a fuel assembly in the lattice calculation, and to produce the group constants for the node of the core calculations. In this process, the details of lattice geometry are taken into account. One also needs to consider the environmental effects when using the group constants in the core calculations (Chinaka, et al., 2015). This arises since the lattice calculations normally use reflective boundary conditions, and the effect of neighbouring nodes is not considered. Other quantities such as diffusion coefficients are also required in core calculations using diffusion theory.

3.9 Burn-Up

Fuel burn-up refers to the consumption of fuel material. In a neutron flux the fuel undergoes various nuclear reactions and decays, which lead to the formation of new isotopes. The detailed burn-up analysis predicts the change in the isotopic fuel composition, leading to the production of a variety of transuranic elements in the actinide series of the periodic table, as the function of time and space.

There are three main processes, which have to be monitored during reactor operations. They are:

1. The decrease in fissile isotope concentration due to fission and transmutation;
2. The fission products that are produced in the fission events; and

3. The fertile nuclei that are converted to fissile isotopes in the series of transmutations and decays.

All these processes influence the reactor reactivity. For a reactor operating on the uranium cycle, the isotopic concentrations are described by (Stacey, 2007).

$$\begin{aligned}
\frac{\partial n^{24}}{\partial t} &= -\sigma_a^{24} \phi n^{24} \\
\frac{\partial n^{25}}{\partial t} &= \sigma_\gamma^{24} \phi n^{24} - \sigma_a^{25} \phi n^{25} \\
\frac{\partial n^{26}}{\partial t} &= \sigma_\gamma^{25} \phi n^{25} - \sigma_a^{26} \phi n^{26} + \lambda_{ec}^{36} n^{36} \\
\frac{\partial n^{27}}{\partial t} &= \sigma_\gamma^{26} \phi n^{26} + \sigma_{n,2n}^{28} \phi n^{28} - \lambda^{27} n^{27} \\
\frac{\partial n^{28}}{\partial t} &= -\sigma_a^{28} \phi n^{28} \\
\frac{\partial n^{29}}{\partial t} &= \sigma_\gamma^{28} \phi n^{28} - (\lambda^{29} + \sigma_a^{29} \phi) n^{29} \\
\frac{\partial n^{36}}{\partial t} &= \sigma_{n,2n}^{37} \phi n^{37} - (\lambda^{36} + \sigma_a^{36} \phi) n^{36} \\
\frac{\partial n^{37}}{\partial t} &= \lambda^{27} n^{27} - \sigma_a^{27} \phi n^{37} \\
\frac{\partial n^{38}}{\partial t} &= \sigma_\gamma^{37} \phi n^{37} - (\lambda^{38} + \sigma_a^{38} \phi) n^{38} \\
\frac{\partial n^{39}}{\partial t} &= \lambda^{29} n^{29} - (\lambda^{39} + \sigma_a^{39} \phi) n^{39} \\
\frac{\partial n^{48}}{\partial t} &= \lambda^{38} n^{38} - \sigma_a^{48} \phi n^{48} \\
\frac{\partial n^{49}}{\partial t} &= \lambda^{39} n^{39} - \sigma_a^{49} \phi n^{49} + \sigma_\gamma^{48} \phi n^{48} \\
\frac{\partial n^{40}}{\partial t} &= \sigma_\gamma^{49} \phi n^{49} - \sigma_a^{40} \phi n^{40} + \sigma_\gamma^{29} \phi n^{29} + \sigma_\gamma^{39} \phi n^{39} \\
\frac{\partial n^{41}}{\partial t} &= \sigma_\gamma^{40} \phi n^{40} - (\lambda^{41} + \sigma_a^{41} \phi) n^{41} \\
\frac{\partial n^{42}}{\partial t} &= \sigma_\gamma^{41} \phi n^{41} - \sigma_a^{42} \phi n^{42} \\
\frac{\partial n^{43}}{\partial t} &= \lambda^{42} n^{42} - (\lambda^{43} + \sigma_a^{43} \phi) n^{43} \\
\frac{\partial n^{51}}{\partial t} &= \lambda^{41} n^{41} - (\lambda^{51} + \sigma_a^{51} \phi) n^{51}
\end{aligned}$$

$$\begin{aligned}\frac{\partial n^{52}}{\partial t} &= \sigma_{\gamma}^{51} \phi n^{51} - \sigma_a^{52} \phi n^{52} \\ \frac{\partial n^{53}}{\partial t} &= \lambda^{43} n^{43} - \sigma_a^{53} \phi n^{53} + \sigma_{\gamma}^{52} \phi n^{52} .\end{aligned}\tag{3.15}$$

In Equation 3.17, the two-digit superscript convention for identifying isotopes has been adopted. The first digit is the last digit in the atomic number and the second digit is the last digit in the atomic mass (Stacey, 2007). For example, for n^{24} , the 2 comes from the atomic number 92 and the 4 comes from atomic mass 234, giving the isotope ^{234}U . The same applies to n^{25} , where the 2 comes from atomic number 92 and the 5 comes from atomic mass 235, giving the isotope ^{235}U .

The general burn-up equation satisfied by a fission product species j is given as:

$$\frac{dn_j}{dt} = \text{production rate} - \text{absorption rate} - \text{decay rate}$$

and mathematically as (Stacey, 2007):

$$\frac{dn_j}{dt} = \gamma_j \Sigma_f \phi + \sum_i (\lambda^{i \rightarrow j} + \sigma^{i \rightarrow j} \phi) n_i - (\lambda^j + \sigma_a^j \phi) n_j \tag{3.16}$$

where n_j is the isotope being produced, t is time, Σ_f is the macroscopic fission cross-section, γ_j is the fraction of fission events that produces a fission product species j , $\lambda^{i \rightarrow j}$ is the decay rate of isotope i to produce isotope j (beta decay, alpha decay, etc.), $\sigma^{i \rightarrow j}$ is the transmutation cross-section for the production of isotope j by neutron capture in isotope i , n_i is the isotope undergoing transmutation, λ^j is the decay rate of isotope j , σ_a^j is the absorption cross-section of isotope j , ϕ is the neutron flux, and σ_a^j is the cross-section for the destruction of isotope j by neutron absorption in isotope j .

In order to predict the evolution of the final isotopic composition of the fuel and to assess criticality of the nuclear system, one has to analyze the burn-up chains for many types of isotopes. For this purpose, computer codes are used.

In practice, some burn-up computations begin by dividing the time scale into a number of intervals of length Δt . The multi-group flux and k_{∞} are then solved at $t = 0$, the beginning of the first interval - that is, beginning-of-life of the core (BOL). It is then assumed that the multi-group fluxes computed for t_0 remain constant through the first interval to time $t_1 = t_0 + \Delta t$. These fluxes are used to compute the distribution of fuel, converted material, and poisons at t_1 (Lamarsh & Baratta, 2012). According to Wagner and DeHart's report (Kepisty, et al., 2016), 18 to 24 intervals are recommended for studies of the PWR and BWR fuel assemblies.

Since the fissile content of the fuel in a thermal reactor decreases with burn-up with a corresponding increase in fission products, the k_{eff} (core multiplication constant) decreases. In order to assure the operation at the desired power level during the whole reaction cycle the initial core must provide a sufficient amount of excess reactivity. This excess reactivity is then normally offset by diluting boron into the water, and as burn-up progresses, the decrease in the excess reactivity is normally compensated by the simultaneous reduction of the boron concentration in water. This excess reactivity depends on the fuel enrichment, fuel load and loading pattern (Stacey, 2007).

CHAPTER 4 METHODOLOGY

In this chapter, procedures that were followed when developing the models of the selected fuel assemblies studied in this dissertation, are explained.

This chapter is divided into five sections. The first section describes the development of the HEADE and the Serpent models of the simplest fuel assembly slice which does not have a spacer grid. The second section describes the HEADE and Serpent calculations. The third section describes how a spacer grid was added to the same fuel assembly slice and its effects investigated. The fourth section deals with changing the fuel enrichment in the fuel assembly slice in order to determine the effects thereof. In the fifth section, the study of other models of selected fuel assemblies is explained.

4.1 Development of the HEADE and the Serpent Models for the Standard Fuel Assembly

The beginning-of-life/fresh fuel core conditions were used to build the model at steady state conditions. The following assumptions were made during the development of the model:

- i. No temperature feedback ($T = 300\text{K}$);
- ii. A white boundary condition for neutrons as allowed in HEADE was assumed; and
- iii. Not all BEAVRS defined isotopes are available in the HEADE library, therefore some isotopes had to be represented in their elemental form, for example, oxygen was represented as 'O' rather than O-16, O-17, and O-18.

As a starting point, fuel assembly J9 was chosen from the loading pattern shown in Figure 2-5 due to it being one of the simplest fuel assemblies in the BEAVRS core as described in Section 2.2 of this dissertation. The axial position was chosen at 365.76 cm from the bottom of the core, which did not contain any spacer grids. During the development of the model, the lattice had fuel pins and guide tubes that match the fuel assembly given in Figure 11 in the BEAVRS handbook (Horelik & Herman, 2013), herein shown as Figure 2-6. The corresponding HEADE fuel assembly input and material maps model are shown in Figure 4-1 together with an inset of the fuel pin.

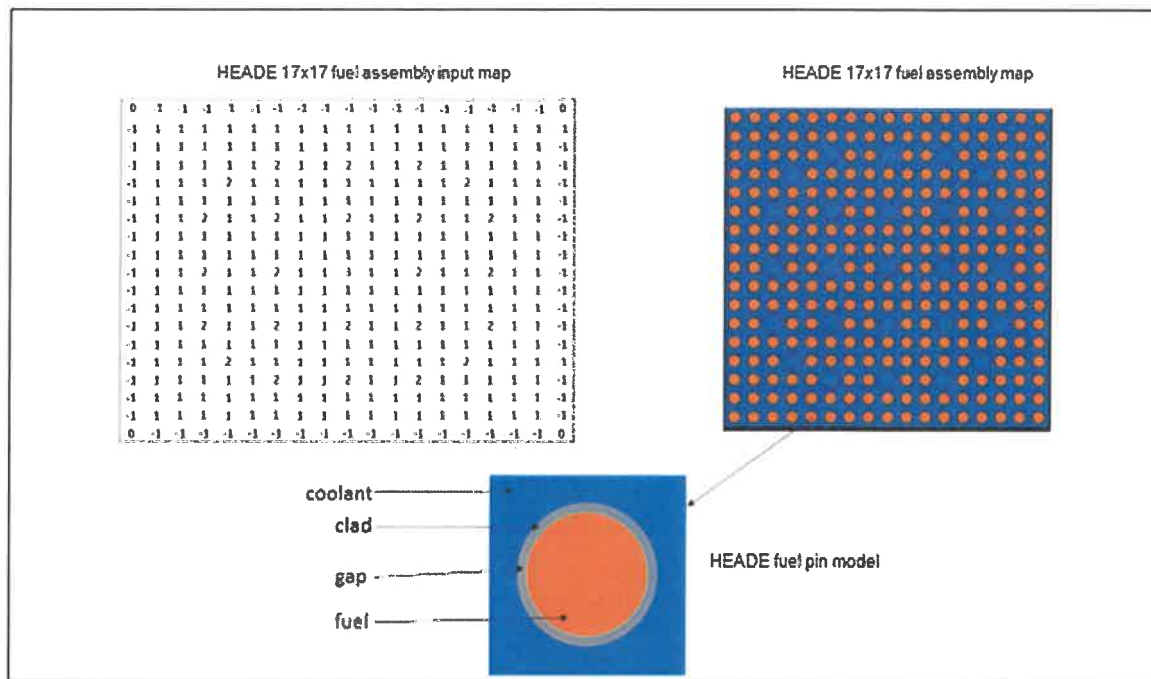


Figure 4-1: A HEADE geometry and materials outline for the 17 x 17 fuel assembly

The number '1' in the fuel assembly input map represents a fuel pin while the number '2' represents a guide tube. The HEADE input model was completed by inserting the parameters from Table 2-1, that is, power, pressure, enrichment, etc. into the input model.

As these parameters were being inserted in the model, the materials, their sequence and their radial specifications were adjusted to correspond with those of the fuel pin and the empty guide tube given in Figure 2-8 and Figure 2-9 respectively. The operating pressure of 2250 psia given in the BEAVRS handbook was converted to 155129.96 kPa and ultimately to 155.129 bars as required by the HEADE code. The radial geometry included radii of the fuel pin, empty guide tube and bare instrument tube. The radii of the fuel pin and those of an empty guide tube are as shown in Figure 2-8 and Figure 2-9 respectively. At this stage, it is brought to the attention of the reader that the radial geometry of an empty instrumentation tube is the same as that of an empty guide tube as given above. The axial specifications, i.e. the length of the fuel rod and the active fuel length of the fuel rod, and those of the empty guide tube and instrument tube were also inserted in the model from Table 2-1. The benchmark specifications, as given in Appendix A, were used to define a material card and the resultant model gave the first BEAVRS fuel assembly model which is referred to as a **standard model**.

The reference Serpent model was constructed directly from the material and geometric description given in the benchmark specification document, with no approximations in either. The model was developed and then provided to an independent Serpent expert user for review. In order to ensure consistency with HEADE, all calculations were run with a point-wise cross-section library based on JEFF 2.2 and to a Monte Carlo accuracy of approximately 10 pcm in reactivity. Depletion was also performed with Serpent in order to compare burn-up dependent quantities with HEADE, and was performed using a predictor-corrector method on the same time discretization as was used in the HEADE depletion calculations.

4.2 Burn-Up

For the burn-up calculation, the first model is used which consists of the following: 1.6 % fuel enrichment, empty guide tubes and instrumentation tube and no spacer grids. With this model, a small area inside the core is simulated, where properties of the system such as moderator density can be assumed to be constant. This approach is sufficient for observing eventual systematic discrepancies of the burn-up procedure (Kepisty, et al., 2016).

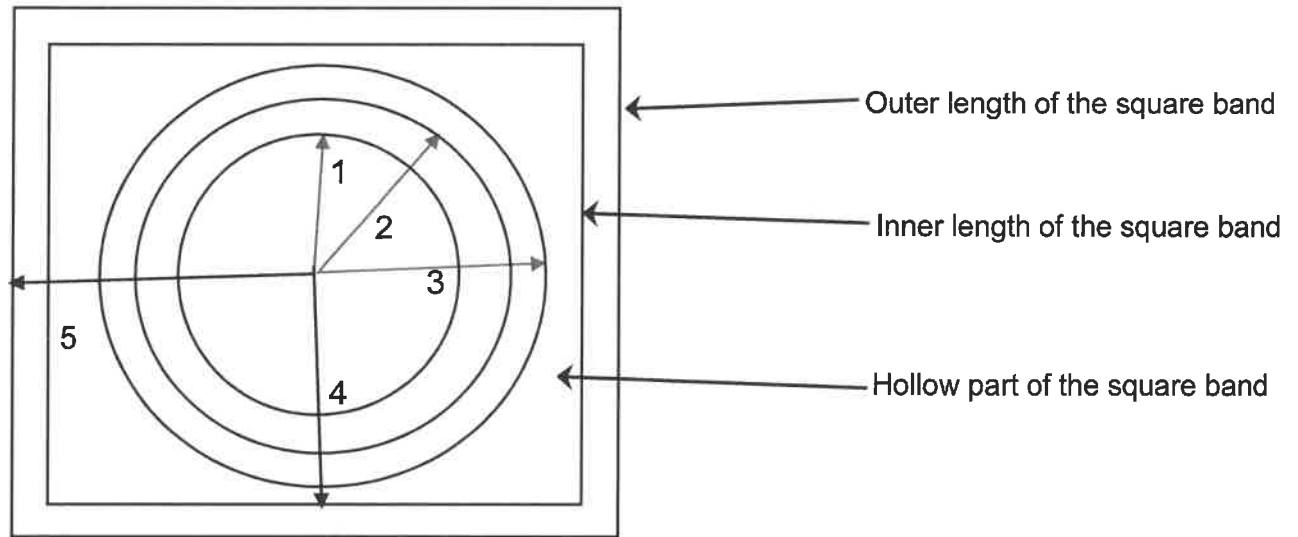
The fuel was burnt to about 43 GWD/tU and the power of the system was set to the core average assembly power value of 1885.54 MW. Results concerning a change of isotopic composition are presented using the relative difference of mass. The evolution of k_{inf} and that of the following isotopes as a function of burn-up was investigated, ^{235}U ; ^{238}U ; ^{239}Pu ; ^{135}Xe ; and ^{149}Sm . The results of this process are shown and discussed in Section 5.2 of this dissertation.

4.3 Adding a Spacer Grid to a Fuel Assembly

In order to include the spacer grid to the standard model developed in Section 4.1, the model was adapted as follows:

The spacer grid used in this model, is assumed to be a square shaped band with inner and outer dimensions as shown in Figure 4-2. This assumption is made in the BEAVRS benchmark to ease the modelling. As there is no provision in HEADE to include a square

configuration around a circular one, the spacer grid was represented as an annular disc with inner and outer radii. The outer radius of the annular disc was taken to be half the length of the outer length of the square spacer grid band. In order to determine the inner radius of the annular disc, the area of the square spacer grid band had to be conserved and the inner radius was determined using Figure 4-2.



Arrow	Radius (cm)	Material
1	0.39218	Fuel
2	0.40005	Helium
3	0.45720	Zircaloy
4	0.60978	Water
5	0.62992	Zircaloy

Figure 4-2: Fuel pin-cell geometry for the Zircaloy intermediate spacer grid

Area of the square band = Area of annular disc

Area of the square band:

$$A_{h\text{-square band}} = (\text{Outer length})^2 - (\text{inner length})^2$$

$$= 0.099870232 \text{ cm}^2$$

Area of annular disc:

$$A_{h\text{-disc}} = \pi (R_{\text{outer}})^2 - \pi (R_{\text{inner}})^2$$

$$A_{h\text{-square band}} = \pi (0.62992)^2 - \pi (R_{\text{inner}})^2$$

$$R_{\text{inner}} = 0.604160181 \text{ cm}$$

The k_{inf} for the **standard model** (without the spacer grid), which was taken to be **Model A**, was calculated. It must be kept in mind that the coolant in this case was borated water

(H₂O + B). In order to keep the model simple so that only the effect of adding the spacer grid could be observed, the model was adjusted by removing Boron from the coolant (H₂O + B) to be left with water (H₂O) as coolant. This was taken to be **Model B**. The k_{inf} for this model was also calculated. Model B was then adjusted to **Model C** by creating a water spacer grid. The water spacer grid was created by increasing the number of radii around the fuel pin in the model to include the spacer grid radii as calculated above. The k_{inf} for this model was also determined and recorded. **Model C** was adjusted to create **Model D** by replacing the water spacer grid (water) with Zircaloy-4 spacer grid. The k_{inf} for the model was also determined and recorded. **Model D** was then adjusted to create **Model E** by adding Boron back into the water to have the coolant as borated water (H₂O + B).

Table 4-1: Fuel assemblies observed during spacer grid investigation

Fuel Assembly	Boron in Coolant	Water Spacer Grid	Zircaloy-4 Spacer Grid
Model A (Standard Model)	Y	N	N
Model B (same as Model A but without boron in water)	N	N	N
Model C (same as Model B but with water spacer grid)	N	Y	N
Model D (same as Model B but with Zircaloy-4 spacer grid)	N	N	Y
Model E (same as Model D but with boron in water)	Y	N	Y

The results of this investigation are tabulated in Table 5-3 and the group constants obtained from the model of the fuel assembly with the spacer grid are tabulated in Table 5-4.

4.4 Changing Enrichment

The models for other fuel assemblies were built from that of the standard fuel assembly built in Section 4.1. The models that were built were those where enrichment has changed. The enrichment in the model was changed from 1.6 % to 2.4 % to match fuel assembly M12. Changing fuel enrichment, changes the fuel density slightly, therefore the fuel density of 10.31341 g/cc had to be changed to 10.29748 g/cc and the model was run.

The enrichment in the model was again adjusted to a new value of 3.1 % from 2.4 % to match fuel assembly R9. The fuel density of 10.29748 g/cc had to be changed to 10.30166 g/cc and the model was run.

The intention with the enrichment change was to observe the effects on the power and flux profiles. The models were run and the results are discussed in Section 5.4 of this document.

4.5 Adding Burnable Poison, Control Rods, Instrument Pin

In this section, burnable poisons, control rods and lastly the instrument tube pin was added to the fuel assembly in consecutive steps. The steps followed in building the models are outlined below.

Fuel assembly K9 was chosen from the loading pattern as shown in Figure 2-5 in which the enrichment was 2.4 %. The fuel assembly has 12 burnable absorber pins and are configured as shown in Figure 2-7. The HEADE input file for the fuel assembly with empty guide tubes (from Section 4.1) was changed to match the configuration in Figure 2-7. The number of radii, the radii sizes and the materials were changed to correspond with those in Figure 2-12. The model was run and the results are recorded in Table 5-7 and are discussed in Section 5.4.2 of this document.

Fuel assembly K8 was chosen from the loading pattern as shown in Figure 2-5 with an enrichment of 1.6 %. This fuel assembly has all guide tube positions filled with the control rod pin-cells with the exception of the centre tube reserved for the instrument tube. During the development of the HEADE model with control rods, the HEADE input file for the fuel assembly with empty guide tubes (from Section 4.1) was changed to so that all guide tube positions are filled with control rods. The number of radii, the radii sizes and the materials were changed to correspond with those in Figure 2-10. The model was run and the results are recorded in Table 5-7 and discussed in Section 5.4.2 of this document.

Fuel assembly J7 was chosen from the loading pattern as shown in Figure 2-5. This fuel assembly has no burnable absorber pins, meaning that all guide tube positions were empty with the exception of the centre tube which was now filled with the instrument pin. The enrichment was 1.6 %. The HEADE input file for the fuel assembly with empty guide

tubes (from Section 4.1) was changed so that the centre position is filled with the instrumentation pin. The number of radii, the radii sizes and the materials were changed to correspond with those in Figure 2-11. The model was run and the results are recorded in Table 5-7 and discussed in Section 5.4.2 of this document.

CHAPTER 5 RESULTS

This chapter presents the results that were obtained from running the models which were developed as described in Chapter 4. These results are discussed in comparison with the work of other researchers. The first section of this chapter discusses comparison of the burn-up results of the 2-group HEADE model with the results of the 2-group Serpent model for the standard model. The second section discusses other results obtained from HEADE. The third section discusses the results of fuel assembly J9, the standard model, surrounded with a spacer grid. A comparison with Serpent at BOL is also performed for this assembly. The fourth section discusses the results obtained from HEADE when fuel enrichment was changed while the fifth section discusses the HEADE results of other non-standard fuel assemblies (as described in Section 4.5).

5.1 Burn-Up

This section deals with the comparison of the HEADE burn-up results with the Serpent burn-up results for the standard model. The comparison between HEADE and Serpent is limited to a subset of parameters which could be extracted from Serpent. These parameters which include burn-up, k_{inf} and mass of ^{235}U are tabled in Appendix C in this document. A series of further parameters are extracted and reported only from HEADE. These are reported in Section 5.2 of this dissertation.

5.1.1 Multiplication factor

Table 5-1: Comparison of HEADE and Serpent group constants

Code	k_{inf}	Thermal < 0.625 eV			Fast > 0.1 MeV		
		Σ_a (cm^{-1})	Σ_f (cm^{-1})	D	Σ_a (cm^{-1})	Σ_f (cm^{-1})	D
HEADE Standard FA	1.00818	7.97E-02	4.04E-02	3.26E-01	8.54E-03	1.87E-03	1.45E+00
Serpent	1.01156	7.83E-02	3.82E-02	4.86E-01	7.81E-03	1.68E-03	1.52E+00
Difference	- 0.00338	0.0014	0.0022	-0.1600	0.0007	0.0002	-0.0700
% Difference		1.8	5.6	-39.4	8.9	10.7	-4.7
Δk_{inf} (pcm)	-0.338						

Table 5-1 tabulates the infinite multiplication factor as well as the group constants obtained from both HEADE and Serpent for the standard model. The k_{inf} values for the initial conditions, i.e. before burn-up or at BOL, that were produced by both codes are compared. It can be seen that the difference between the two k_{inf} values for the initial conditions is more or less 339 pcm in magnitude, which is about 0.34 %. This is indicative of the effectiveness of a HEADE multi-group calculation. HEADE is a multi-group calculation whereas Serpent is a continuous energy Monte-Carlo calculation. In a similar study in which the High Temperature Gas-cooled Reactor (HTGR) was studied, differences in the multiplication constant between the CE and MG KENO calculation were observed to be 340 pcm (Gehin J, et al., 2010). A difference in the multiplication constant using codes of different methodology can therefore be expected.

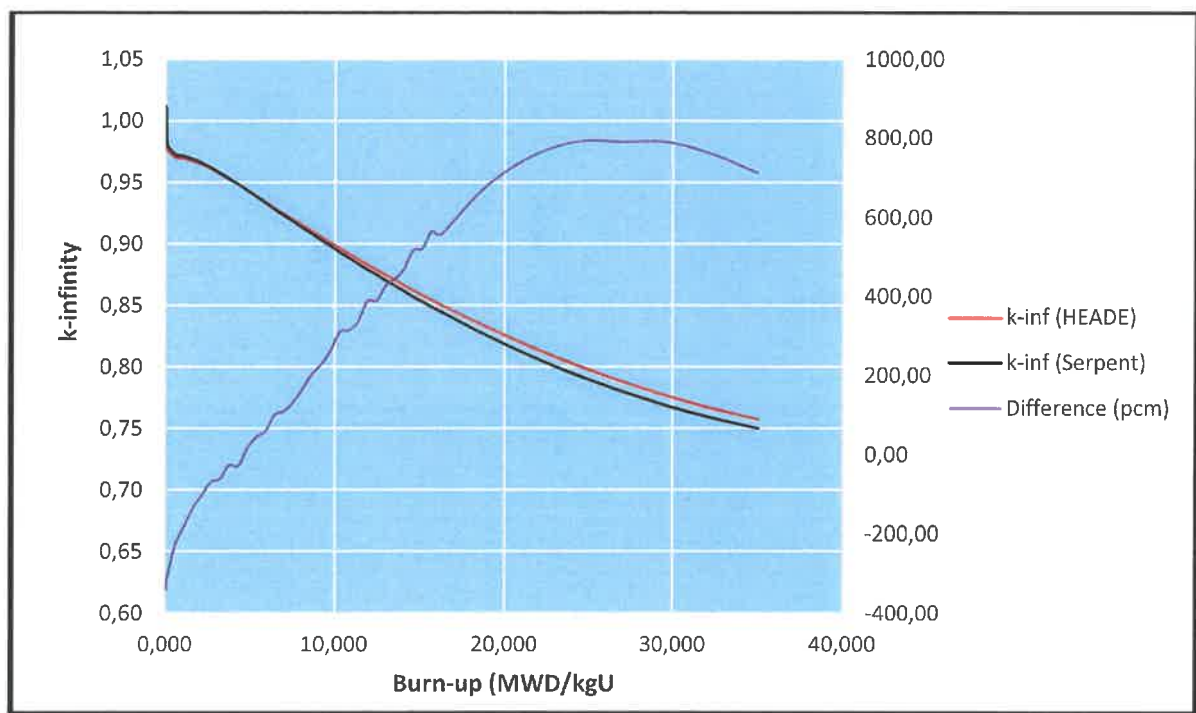


Figure 5-1: Comparison of HEADE and Serpent k-infinity

The behaviour of k_{inf} during fuel burn-up as obtained from both HEADE and Serpent is shown in Figure 5-1. As expected, there is a rapid drop in k_{inf} at the early stage of burn-up time due to the initial build-up of xenon. It can also be seen that for both codes the graphs of k_{inf} during burn-up are very similar, as the difference in k_{inf} between the two codes ranges between -341 and 792 pcm. Given the expected difference when using the multi-group HEADE code with that of the continuous energy Serpent code as discussed above, the similarity in the infinite multiplication factor as a function of burn-up implies that the two codes are compatible with regard to reactivity during fuel burn-up. This kind of behaviour

of the k_{inf} during burn-up has been confirmed by (Yu, et al., 2015). It can also be seen that k_{inf} at BOL is 1.00818 while that at EOL is 0.73660 as obtained from HEADE. In terms of infinite lattice calculations, this is a very good comparison given the fact that the two codes used different cross-section libraries.

5.1.2 Group constants

In Table 5-1, a comparison of the group constants produced by both HEADE and Serpent at BOL is also shown. It can be seen that the difference between absorption cross-sections for the two codes in the thermal group is about 2 % and the difference between absorption cross-sections for the two codes in the fast group is about 10 %. It can also be seen that the difference between fission cross-sections for the two codes in the thermal group is about 6 % and the difference between fission cross-sections for the two codes in the fast group is also about 10 %. As mentioned earlier, the 10 % difference needs to be investigated further.

The behaviour of the absorption cross-section from BOL to EOL as obtained from HEADE is depicted in Figure 5-2. It is also noted that the absorption cross-section remains somewhat constant throughout the burn-up time. Depletion calculations are useful for overall fuel cycle analysis.

The graph shows, as would be expected, that more neutron absorption takes place in the thermal group than in the fast group. This is expected, since the microscopic absorption cross-section for isotopes are larger at thermal energies than at fast energies. It is also noted that the absorption cross-section increases with an increase in burn-up and indicates a hardening of the spectrum. This is due to the production of fission products as the fission process occurs which add to the absorption cross-section.

When comparing the diffusion coefficients as tabulated in Table 5-1, it can be seen that the percentage difference for diffusion coefficients is large in the thermal group, about 40 % and smaller in the fast group, about 5 %. A possible explanation is that the manner in which the diffusion coefficient is calculated is different for the two codes. The large percentage difference for the thermal value warrants further investigation. However, since it will mean examination of the source files of both codes, this will be reserved for future study. With the exception of this large percentage difference of the diffusion coefficient in

the thermal group, the percentage differences for the other parameters listed in Table 5-1 were less than 10 %. However, since the production of the macroscopic cross-sections and the diffusion coefficient is required for the nodal core calculation, the effect of these differences can be better appreciated upon completion of such core calculations.

The behaviour of ^{235}U depletion during fuel burn-up as obtained from both HEADE and Serpent is shown in Figure 5-3. It can be seen that for both codes the graphs for the depletion of ^{235}U are very similar in shape. At 0.1 the burn-up starts to increase while the ^{235}U starts to decrease. The difference between the two codes ranges between 0 % and 17 % at EOL. The mass of ^{235}U at BOL was 6829.56 g and it was 259.53 g at EOL, which implies that the 17 % is about 44 g at EOL showing that the ^{235}U mass decreases during fuel burn-up. This results from slightly different spectra and associated plutonium production through the assembly life.

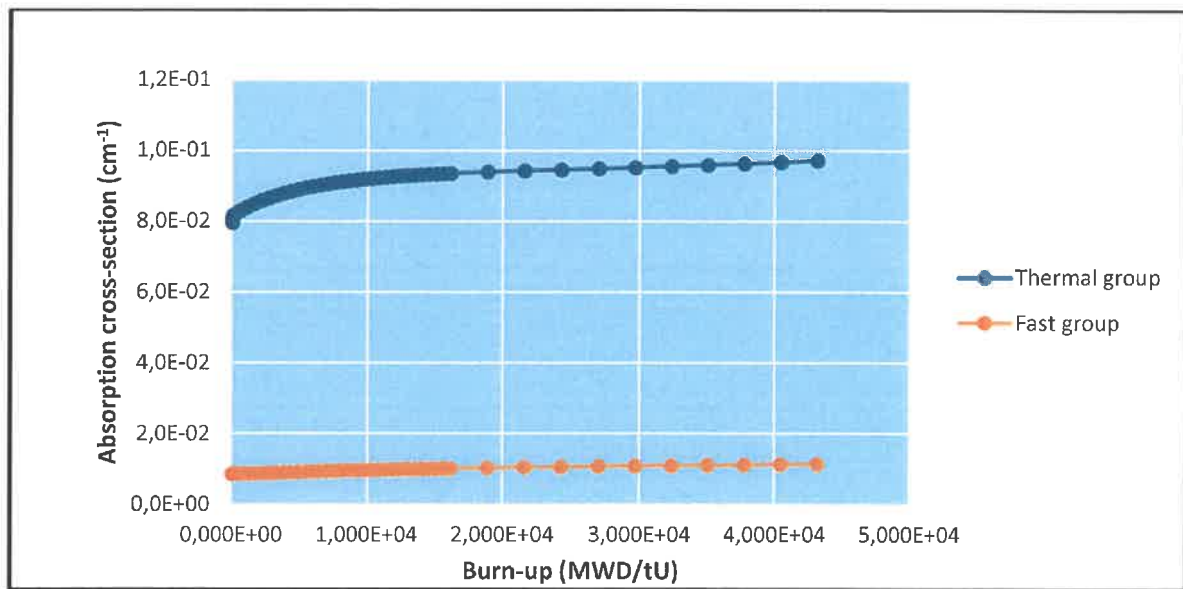


Figure 5-2: Absorption cross-section versus burn-up

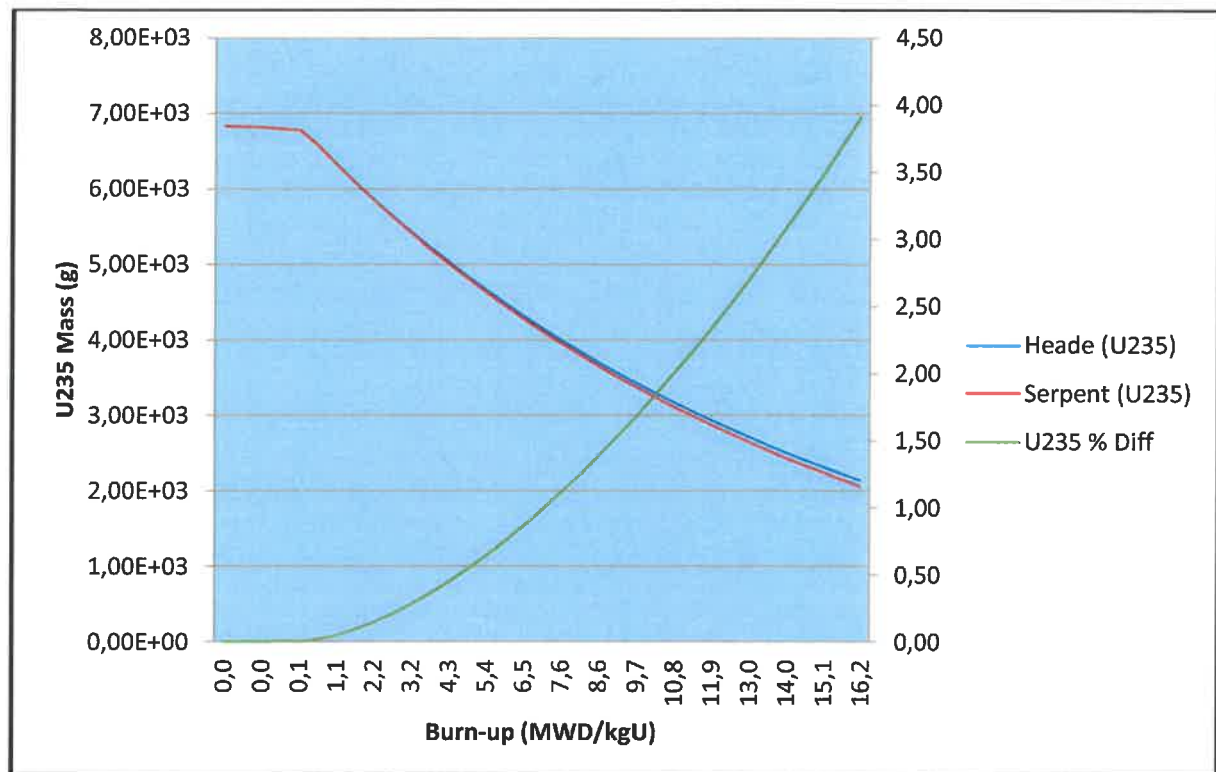


Figure 5-3: U-235 depletion during burn-up

5.1.3 Power

A comparison between power in the different fuel pins as obtained from the two codes at BOL was also made.

Error! Not a valid bookmark self-reference. shows power distribution for one-eighth of the fuel assembly as calculated using the HEADE and the Serpent codes. The power shown in the table is the direct pin-power (not normalized) and is given in units of $1\text{E}+04$ W. A comparison is made between the two codes by calculating the percentage difference in power as calculated by HEADE and Serpent in each of the fuel pins; that difference has also been shown in Table 5-1.

A study in which the full-core pin-power distributions at core mid-plane using the computer codes ARES and 3D Serpent results showed good agreement (Leppänen, et al., 2014). The relative differences were below 1 % in 82 %, and below 2 % in 98 % of all pins. In the current study, it can be seen that the difference in power distribution also ranges between 1 % and 2 % in magnitude. This shows that there is a good comparison between the HEADE and Serpent pin-power calculations.

Table 5-2: Comparison of HEADE and Serpent fuel power maps

0.938	0.942	0.949	0.958	0.967	0.975	0.972	0.972	0.976	HEADE
0.9601	0.9573	0.9602	0.9678	0.9746	0.9807	0.9818	0.9818	0.9842	SERPENT
0.0221	0.0153	0.0112	0.0098	0.0076	0.0057	0.0098	0.0098	0.0082	Δ
2%	2%	1%	1%	1%	1%	1%	1%	1%	% Δ
	0.947	0.959	0.975	0.987	1.008	0.991	0.972	1.007	
	0.9538	0.9620	0.9738	0.9882	1.0066	0.9922	0.9925	1.0070	
	0.0068	0.0030	-0.0012	0.0012	-0.0014	0.0012	0.0205	0	
	1%	0%	0%	0%	0%	0%	2%	0%	
		0.981	1.015	1.028		1.024	1.022		
		0.9797	1.0097	1.0229		1.0188	1.0179		
		-0.0013	-0.0053	-0.0051		-0.0052	-0.0041		
		0%	-1%	0%		-1%	0%		
				1.041	1.040	1.013	1.009	1.029	
				1.0357	1.0305	1.0072	1.0054	1.0224	
				-0.0053	-0.0095	-0.0058	-0.0036	-0.0066	
				-1%	-1%	-1%	0%	-1%	
				1.029	1.040	1.015	1.013	1.031	
				1.0235	1.0322	1.0083	1.0078	1.0240	
				-0.0055	-0.0078	-0.0067	-0.0052	-0.0070	
				-1%	-1%	-1%	-1%	-1%	
						1.035	1.033		
						1.0253	1.0245		
						-0.0097	-0.0085		
						-1%	-1%		
						1.014	1.013	1.032	
						1.0087	1.0089	1.0253	
						-0.0053	-0.0041	-0.0067	
						-1%	0%	-1%	
							1.013	1.032	
							1.0103	1.0266	
							-0.0027	-0.0054	
							0%	-1%	



Figure 5-4 displays the conventional way of showing the power profiles of a fuel assembly and in this case the power profile is that of the standard fuel assembly as obtained from HEADE.



Figure 5-4: Power profile for the standard fuel assembly

5.2 Additional Parameters Obtained from HEADE

The reactor considered in this study operates on the uranium cycle. During the operation of the reactor a number of changes occur in the composition of the fuel. The various nuclei are transmuted and some of the important elements transmuted during fuel burn-up are considered in the discussions below. The elements that are considered are the following: ^{235}U , ^{238}U , ^{239}U , ^{238}Pu , ^{239}Pu , ^{240}Pu , ^{241}Pu , ^{242}Pu , ^{139}Sm and ^{135}Xe . The concentration, as extracted from HEADE results, of some these elements are given in Appendix B in this document.

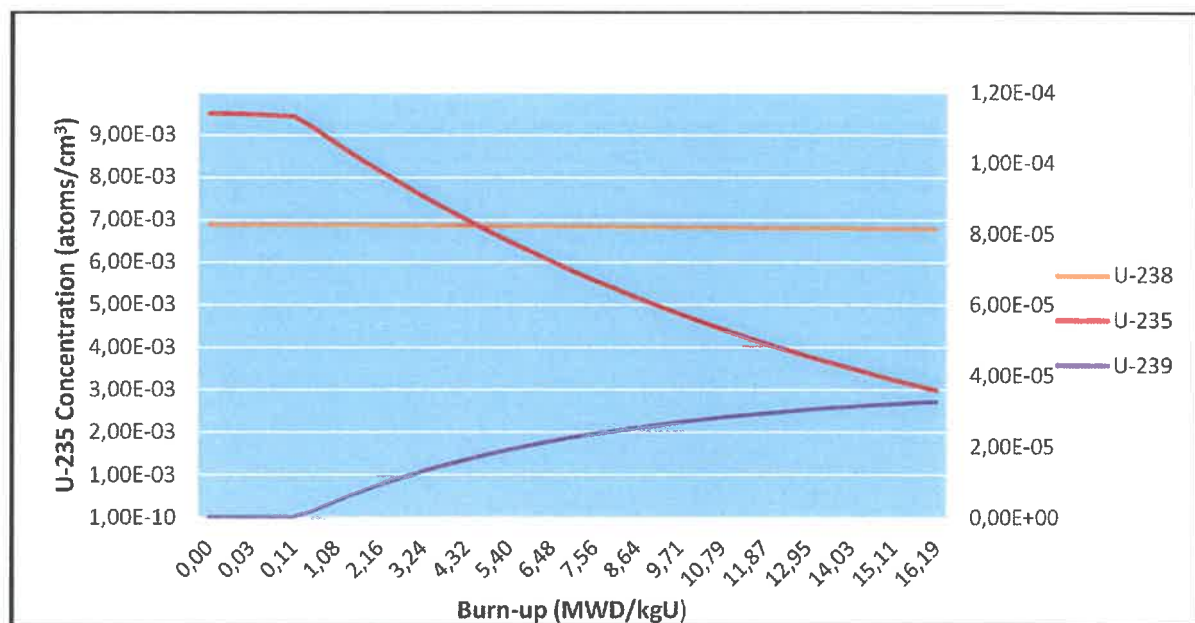


Figure 5-5: Change in concentration of uranium isotopes versus burn-up

One of the isotopes of interest during fuel burn-up is ^{235}U . Attention is brought to the reader that the concentrations of ^{235}U have been plotted on the primary scale while that of ^{238}U and ^{239}U have been plotted on the secondary scale in Figure 5-5. During the reactor operation, the initial ^{235}U will be consumed due to fission and neutron capture processes. This behaviour of ^{235}U is illustrated in Figure 5-5 where the concentration of ^{235}U decreases as a function of burn-up. Transmutation of ^{235}U finally leads to ^{237}Np . Neutron capture in the fertile isotope ^{238}U leads to ^{239}U . Figure 5-5 shows how ^{238}U decreases during burn-up. ^{239}U decays to ^{239}Np and further decays to the fissile isotope ^{239}Pu . The build-up and subsequent decay of ^{239}U is also shown in Figure 5-5 while the build-up of ^{239}Pu is illustrated in Figure 5-6. The build-up of the fissionable isotope ^{239}Pu in turn is transmuted by neutron capture into ^{240}Pu and further into higher actinide isotopes. ^{240}Pu is also built up by the decay of ^{240}U . The various Pu isotopes as a function of burn-up are shown in Figure 5-6. ^{239}Pu and ^{241}Pu are the products of the transmutation-decay chain beginning with the fertile ^{238}U . Further elaboration on the production and removal of Pu with burn-up in UO_2 fuel can be found in (Yu, et al., 2015).

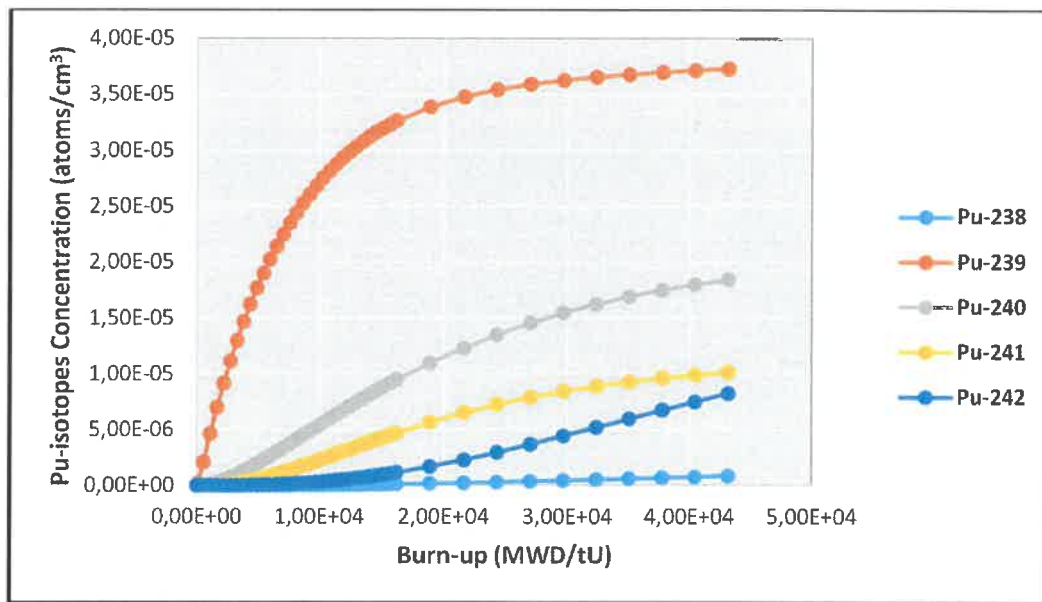


Figure 5-6: Build-up of Plutonium isotopes

During the ^{238}U transmutation-decay process, the actinides are built-up as discussed above. This introduces a fuel reactivity penalty because some of the actinides act primarily as parasitic absorbers.

Another isotope of interest during fuel burn-up is ^{149}Sm because it has a large absorption cross-section. The evolution of ^{149}Sm in the fuel assembly as carried out by HEADE is shown in Figure 5-7. The isotope is not present in the initial fuel composition and is formed during fuel burn-up. In the initial stage, ^{149}Sm concentration increases rapidly for a period of around 13 days (539 MWD/tU) as can be seen in Figure 5-7. This increase in ^{149}Sm concentration is due to the production of ^{149}Sm from the beta decay of the fission product ^{149}Nd . In the initial stage, the production of ^{149}Sm exceeds its removal due to decay and due to neutron capture.

$$\frac{dP}{dt} = \gamma^{Nd} \sum_f \phi - \lambda^P P, \quad \frac{dS}{dt} = \lambda^P P - \sigma_a^S \phi S$$

where S and p refer to ^{149}Pm and ^{149}Sm , respectively.

It can be seen that samarium approaches some equilibrium value from around 26 days (1080 MWD/tU).

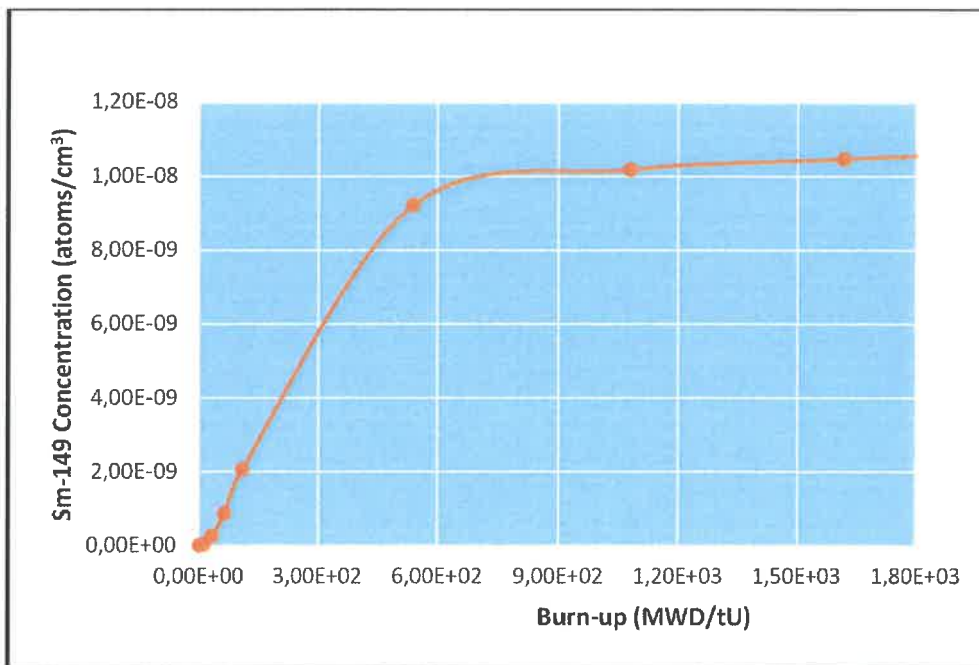


Figure 5-7: Samarium-149 concentration versus burn-up

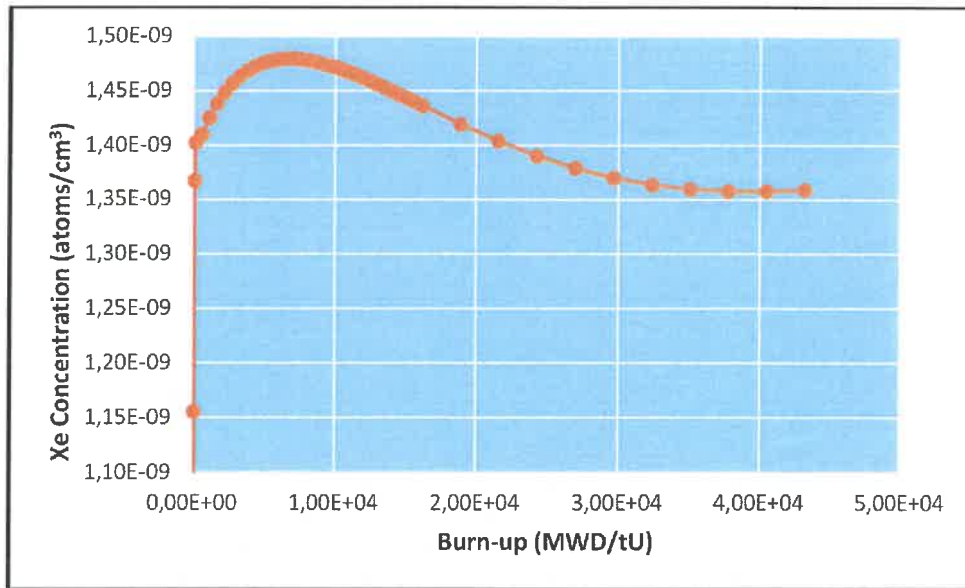


Figure 5-8: Xenon-135 concentration versus burn-up time (540 days)

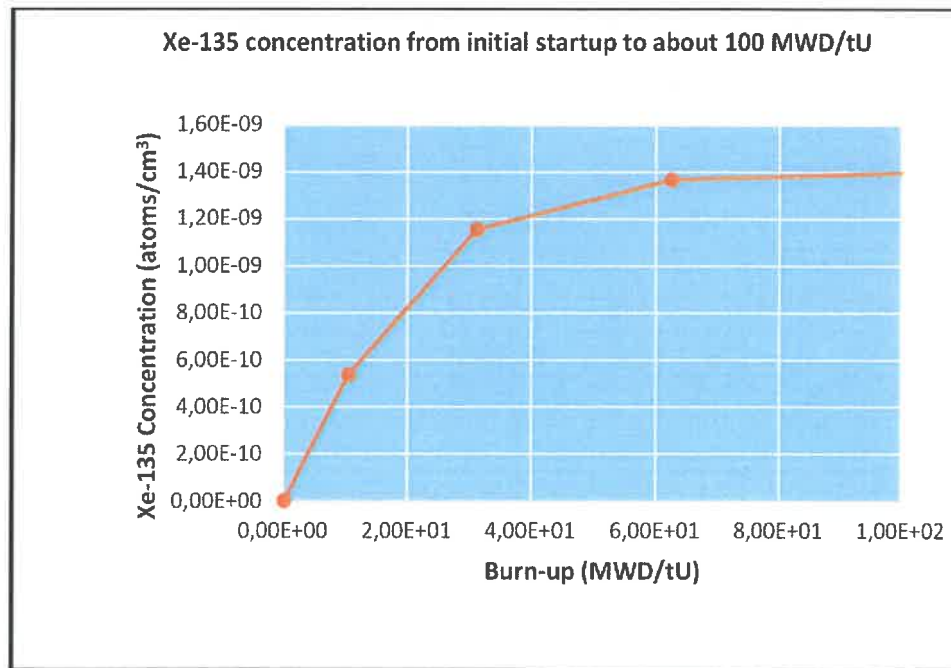


Figure 5-9: Xenon-135 concentration versus burn-up (100MWD/tU)

Figure 5-8 and Figure 5-9 show the evolution of ^{135}Xe in the fuel assembly as carried out by HEADE. The isotope is not present in the initial fuel composition and is formed during reactor operation by being produced directly from fission and from the decay of ^{135}I . In the initial stage, the ^{135}Xe concentration increases for a period of about 2.5 days (107 MWD/tU), as can be seen in Figure 5-8 and Figure 5-9.

The increase in ^{135}Xe concentration is because the production of ^{135}Xe initially exceeds its removal due to decay and neutron capture. It can also be seen that the concentration of

^{135}Xe reaches equilibrium at about 100 MWD/tU (2.5 days' time) from the initial reactor start-up. When comparing the period it takes for the concentrations of ^{135}Xe and ^{149}Sm to reach equilibrium, it can be seen that it takes a shorter period (2.5 days) for ^{135}Xe to reach equilibrium value than it does for ^{149}Sm (26 days or 1080 MWD/tU). HEADE produces results similar to those obtained in (Stacey, 2007).

This concludes the analysis of the standard fuel assembly with HEADE and Serpent. We conclude that HEADE compares favourably with the reference Serpent calculation with reactivity differences of less than 500 pcm for the typical residence time in the core (up to about 40 MWd/kg). Pin-power comparisons are also very good (1 % - 2 %).

Further analysis of the various assembly designs are now conducted with HEADE only. It should however be stated that future work should include a detailed comparison of the remainder of the designs to Serpent reference results, to ensure that the quality of the comparison applies to all required models. A first step in this direction has been performed for the inclusion of a spacer grid into the model and a comparison to Serpent results at BOL is included in Section 5.3.

5.3 Adding a Spacer Grid to a Fuel Assembly Model – Results

When adding a spacer grid volume to the fuel assembly, the water volume will necessarily be decreased. However, if the water is borated, then the amount of boron in the assembly will also decrease; this therefore implies that an extra consideration (i.e. the effect of changing boron) needs to be taken into account. Therefore, it was decided to first remove the boron from the water before adding the spacer grid. The boron could then be re-introduced at the end.

With Model A serving as our reference, it can be noted from Table 5-3 that removing boron from borated water ($\text{H}_2\text{O} + \text{B}$) surrounding the standard fuel assembly (Model A) increases the k_{inf} (Model B) which is as per expectation. Removing boron from the coolant removes neutron absorber material. This allows more of the neutrons to be moderated by the water since there is no competition by boron therefore resulting in an increased reaction with the fuel causing more fission. During the fission reaction the number of neutrons produced is increased, hence the neutron infinite multiplication factor increases.

When examining Models B and C in Table 5-3, it can be noted that by inserting a water spacer grid around the fuel, reactivity is reduced by 58 pcm. This is not as expected since effectively there is still only water present without any physical spacer grid material and the reactivity should have remained the same. In discussion with the code developer (Prinsloo, 2018), a possible reason for this could be attributed to the numerical effect of the discretization of the problem, since this was the effect of adding the water spacer grid.

When examining Models C and D in Table 5-3, it can be noted that by replacing the water spacer grid with a Zircaloy-4 spacer grid, the reactivity increases by 98 pcm. This increase in reactivity was not expected. The volume of the spacer grid (Zircaloy-4) replaces some volume of the water where more neutrons are moderated more effectively than at the Zircaloy-4 spacer grid, therefore a decrease in reactivity was expected. The higher multiplication factor is expected where the fuel assembly does not include a spacer grid, as has been shown experimentally by Tran and Cho (Tran & Cho, 2016).

Again, a possible reason for this unexpected behaviour could be due to numerical effects introduced by defining an additional grid in the solution.

Table 5-3: k_{inf} for fuel assemblies observed during spacer grid investigation

<i>Fuel Assembly</i>	<i>Boron in Coolant</i>	<i>Water Spacer Grid</i>	<i>Zircaloy-4 Spacer Grid</i>	<i>k_{inf}</i>	<i>Δk_{inf} (pcm)</i>
Model A (Standard Model)	Y	N	N	1.00818	-
Model B (same as Model A but without boron in water)	N	N	N	1.20751	19937
Model C (same as Model B but with water spacer grid)	N	Y	N	1.20693	19879
Model D (same as Model B but with Zircaloy-4 spacer grid)	N	N	Y	1.20791	19977
Model E (same as Model D but with boron in water)	Y	N	Y	1.00808	1544

Another possible reason could be that the cell environment in the self-shielding unit cell calculation and the lattice calculation were not precisely maintained when the water spacer grid was modelled. That is, in the self-shielding unit cell calculation, only the water in the space between the cladding and the spacer grid could have been considered whereas in

the lattice calculation both the water between cladding and the spacer grid and that substituted for the spacer grid material was considered.

However, it was noted that, according to Refeat and Louis, the spacer grid would not make such a significant difference (Refeat & Louis, 2016). Therefore, due to the constraint imposed by the scope of this project, and the relatively small differences that were observed in the changes in the multiplication factor, this effect was not investigated further.

In a related topic, (Castle, et al., 2012) studied the impacts that changing the fuel cladding from Al-6061 to Zr-4 would have on the reactor that they studied. From that study, it came out that zirconium has a larger moderating ratio than aluminium, which indicates that zirconium is a more effective neutron moderator. They assumed that the increased moderating ratio of zirconium would likely result in an increase in reactivity, due to the increased effectiveness of neutron moderation and a decrease in neutron absorptions.

The final spacer grid effect observed is when Models A and E in Table 5-3 are compared, Model A being the standard model and Model E being the same model surrounded with a spacer grid. In the Serpent model the reactivity decreases by 70 pcm as expected. This data is not shown in the table. It is noted that by inserting a spacer grid in the HEADE model, the reactivity increased by about 70 pcm which is not the expected results.

Table 5-4: Group constants for the standard fuel assembly with spacer grid and one without

HEADE Models	k_{inf}	Thermal < 0.625 eV			Fast > 0.1 MeV		
		Σ_a (cm^{-1})	Σ_f (cm^{-1})	D	Σ_a (cm^{-1})	Σ_f (cm^{-1})	D
HEADE standard FA	1.00818	7.97E-02	4.04E-02	0.325735	8.54E-03	1.87E-03	1.45E+00
HEADE spacer grid	1.00888	7.68E-02	3.99E-02	0.3544212	8.53E-03	1.84E-03	1.44E+00
% Δ		3.78E+00	1.25E+00	-8.09E+00	1.17E-01	1.63E+00	8.35E-01
Δk_{inf} (pcm)	70.0000						

For the completion of the study on the spacer grids using the present methodology,

Table 5-4 compares some few-group constants of the standard fuel assembly without a spacer grid with those of the fuel assembly which has a spacer grid, the one obtained above.

The percentage differences for the absorption cross-section in the thermal energy group and in the fast group are 3.8 % and 0.1 % respectively. The percentage difference for the fission cross-section in the thermal energy group and in the fast energy group are 1.3 % and 1.6 % respectively. Regarding diffusion coefficients, it is noted that the difference in the thermal energy group is 8.1% while in the fast energy group the difference has a magnitude of 0.8 % with the larger one being that of the fuel assembly with a spacer grid.

Finally, in Table 5-5 the HEADE results for a fuel assembly with spacer grids are compared with the Serpent results for a similar fuel assembly. It can be seen from Table 5-5 that the k_{inf} values obtained from the two codes differ by about 199 pcm. Considering that the two codes use different cross-section libraries and also that HEADE is a multi-group calculation as compared to Serpent which is a continuous energy calculation, the difference in k_{inf} is accepted. However, it should be kept in mind that HEADE had shown unexpected behaviour when the spacer grid was added.

Table 5-5: HEADE and Serpent group constants for the fuel assembly with spacer grids

HEADE Models	k_{inf}	Thermal < 0.625 eV			Fast > 0.1 MeV		
		Σ_a (cm ⁻¹)	Σ_f (cm ⁻¹)	D	Σ_a (cm ⁻¹)	Σ_f (cm ⁻¹)	D
HEADE	1.00888	7.6802E-02	3.9863E-02	3.5442E-01	8.5295E-03	1.8360E-03	1.4404E+00
Serpent	1.01086	7.5333E-02	3.7581E-02	5.1824E-01	7.7974E-03	1.6315E-03	1.4659E+00
%Δ		1.9498E+00	6.0724E+00	-3.1610E+01	9.3884E+00	1.2535E+01	-1.7361E+00
Δ k_{inf} (pcm)	-198.39						

The percentage differences for the diffusion coefficient in the fast energy group is 1.7 % and the percentage differences for the diffusion coefficient in the thermal energy group is 31 %. Regarding absorption cross-sections, it is noted that the difference for the absorption cross-section in the thermal energy group is 2 % while for the fast energy group the difference for the absorption cross-sections is 9.4 %.

5.4 Varying Enrichment

In this section the results of changing the fuel enrichment in the standard fuel assembly are discussed. The fuel enrichment was changed from 1.6 % to 2.4 % and then to 3.1 %. The results are tabulated in Table 5-6.

Table 5-6: Fuel assemblies with 1.6 %, 2.4 % and 3.1 % fuel enrichment

HEADE Models	k_{inf}	Thermal < 0.625 eV			Fast > 0.1 MeV		
		Σ_a (cm^{-1})	Σ_f (cm^{-1})	D	Σ_a (cm^{-1})	Σ_f (cm^{-1})	D
J9 (1.6%)	1.00818	7.963E-02	4.041E-02	3.260E-01	8.535E-03	1.871E-03	1.453E+00
M12 (2.4%)	1.14939	9.653E-02	5.607E-02	3.306E-01	9.119E-03	2.334E-03	1.456E+00
% Δ		-1.74E+01	-2.79E+01	-1.49E+00	-6.36E+00	-1.99E+01	-2.23E-01
Δk_{inf} (pcm)	-16098.8						
R9 (3.1%)	1.23075	1.103E-01	6.866E-02	3.333E-01	9.624E-03	2.731E-03	1.457E+00
% Δ		-2.77E+01	-4.12E+01	-2.27E+00	-1.13E+01	-3.15E+01	-3.44E-01
Δk_{inf} (pcm)	-1511.51						

5.4.1 Infinite multiplication factor (k_{inf})

It is noted that the k_{inf} values of the fuel assemblies, M12 and R9, for which the fuel enrichment was increased from 1.6 % (of the J9 fuel assembly) to 2.4 % and 3.1 % respectively, increased as enrichment was increased. Increased enrichment implies that there are more ^{235}U atoms available in the fuel. More ^{235}U atoms imply that there are more fission reactions that take place for the same number of incident neutrons available for fission to take place meaning that more ^{235}U is being burnt. It is known that two of the primary determinants of the thermal reactor core multiplication are the fuel enrichment and the volume ratio of moderator to fuel. The multiplication increases monotonically with enrichment.

5.4.2 Group constants

In this subsection the group constants as obtained from HEADE when the enrichment in the fuel assemblies was changed are discussed. Table 5-6 shows the group constants of the fuel assemblies that have 1.6%; 2.4% and 3.1% fuel enrichments.

5.4.2.1 *Absorption cross-section (Σ_{abs}):*

The absorption cross-section is higher in the thermal energy group than in the fast energy group. This is expected, since the microscopic absorption cross-section for isotopes are larger at thermal energies than at fast energies. It is also noted that the absorption cross-section increases in both the fast and the thermal energy groups as the fuel enrichment is increased as is expected. Since the fission process is an absorption process, increasing the number of fissile atoms will therefore increase the macroscopic absorption cross-section.

5.4.2.2 *Fission cross-section (Σ_f):*

The fission cross-section is higher in the thermal energy group than in the fast energy group. It is also noted that the fission cross-section increases in both the fast and the thermal energy groups as the fuel enrichment is increased as is expected.

5.4.2.3 *Diffusion coefficient (D):*

The diffusion coefficient is larger in the fast energy group than in the thermal energy group. It is also noted that the diffusion coefficient increases in both the fast and the thermal energy groups as the fuel enrichment is increased, although by a small margin.

These expected results in the above sub-sections including this one therefore add to assurance that the models that were developed are correct.

5.4.3 Power profiles

One-eighth of the combined power map of the fuel assemblies with varying fuel enrichment is shown in Table 5-7. In Figure 5-10, the power profiles in the first row of Table 5-7 are illustrated. It is noted that for the pins that are near the edge of the fuel assemblies, the power is lower while there is an increase as the pins that are towards the middle of the fuel assembly are considered. This implies a power tilt in the assembly from out to in.

Table 5-7: 1/8 of the power map of direct power for the fuel assemblies with varying fuel enrichment

1.027	1.031	1.039	1.049	1.059	1.067	1.064	1.064	1.068	1.6% Enrich
1.015	1.020	1.029	1.040	1.051	1.061	1.057	1.057	1.062	2.4% Enrich
1.008	1.013	1.022	1.035	1.046	1.057	1.052	1.052	1.058	3.1% Enrich
	1.037	1.050	1.067	1.081	1.103	1.085	1.084	1.102	
	1.027	1.042	1.062	1.078	1.105	1.083	1.082	1.105	
	1.021	1.037	1.058	1.076	1.108	1.081	1.080	1.107	
		1.074	1.111	1.125		1.121	1.119		
		1.071	1.117	1.133		1.127	1.125		
		1.068	1.120	1.139		1.131	1.129		
				1.140	1.138	1.109	1.105	1.126	
				1.150	1.147	1.110	1.106	1.132	
				1.156	1.153	1.110	1.106	1.136	
					1.127	1.138	1.111	1.109	1.129
					1.132	1.147	1.113	1.110	1.136
					1.136	1.153	1.113	1.110	1.141
							1.133	1.131	
							1.140	1.138	
							1.145	1.142	
							1.110	1.109	1.130
							1.111	1.110	1.137
							1.111	1.110	1.142
								1.109	1.130
								1.110	1.137
								1.110	1.141

Guide Tube

Instrument Tube

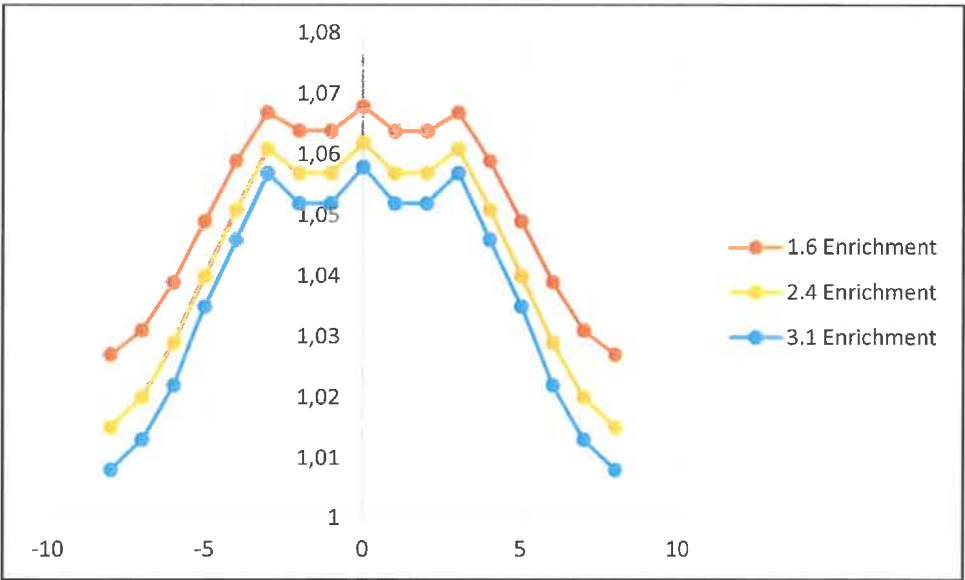


Figure 5-10: Power profiles for row 1 in Table 5-7

5.5 Instrument Pin, Burnable Poison and Control Rods

The models that were built for consideration in this section were the following: burnable poison pins were added to the fuel assembly; control rods were added to the fuel assembly and lastly the instrument tube pin was added to the fuel assembly.

In each model, the self-shielding of the materials in the pins containing UO_2 could only be taken into account, using the method as outlined in Section 5.3. This therefore meant that the treatment of the materials in the instrumentation pin, burnable poison pin and control rods required further investigation. In particular, those materials which have strong resonances in the resonance regions should be given attention.

However, this part of the study was still carried out, since one of the aims of the study was to develop models in which all the elements of the fuel assembly could be modelled in HEADE. The aim is therefore partly achieved since the material and geometry characterization of the complete fuel assembly have been achieved.

It was also considered to be of academic interest to note the effects that each of these different pins had on the results, even though these results cannot be considered to be finalized at this stage of the project on establishing the use of HEADE in PWR applications. The results of the individual changes to the fuel assembly are discussed below.

Table 5-8: 1.6 % enriched fuel assemblies. Empty guide tubes, burnable poison, control rods, instrument tube

HEADE Models		Thermal < 0.625 eV			Fast > 0.1 MeV		
	k_{inf}	Σ_a (cm^{-1})	Σ_f (cm^{-1})	D	Σ_a (cm^{-1})	Σ_f (cm^{-1})	D
Standard FA	1.00818	7.97E-02	4.04E-02	3.26E-01	8.54E-03	1.87E-03	1.45E+00
Burnable poison	0.89138	9.29E-02	4.73E-02	2.71E-01	3.62E-03	2.87E-03	2.45E+00
Control rods	0.30208	9.20E-02	4.68E-02	2.73E-01	3.70E-03	2.97E-03	2.45E+00
Instrument tube	0.95514	9.35E-02	4.76E-02	2.70E-01	3.63E-03	2.91E-03	2.45E+00

It can be noted that the absorption cross-section increased in the thermal groups as changes were made to the fuel assemblies. It can also be noted that the fission cross-section is higher in the thermal energy groups of the fuel assemblies and it is the lower in the fast energy groups for all the changes that were made.

Control rods caused flattening of the flux at the control rod position thereby raising the power in the pins away from the control rod position since the total power in the fuel assembly is kept constant.

Table 5-9 shows the power distribution for the top one-eighth of the top left hand quadrant of the power map of all the fuel assemblies mentioned in Table 5-8. It is noted that the power is the highest in the fuel pins that are away from the control rod position in the fuel assembly with control rods. This could be due to the control rod flattening the flux at the control rods position thereby raising the power in the pins away from the control rod positions since the total power in the fuel assembly is constant.

In order to give a quantitative sense to the numbers shown in control, the powers for the fuel pins in the third column of two pairs of fuel assemblies, viz. fuel assembly with empty guide tubes against fuel assembly with burnable poison, and fuel assembly with empty guide tubes against fuel assembly with control rods, are represented in Figure 5-11 and Figure 5-12 respectively.

In Figure 5-11 it can be seen that the two power profiles differ, with the largest difference for the positions around burnable poison positions where the power has decreased. This is due to the burnable poison being in the positions where there was moderator therefore reducing the fission that could have taken place.

Table 5-9: Power distribution for 1/8 of the fuel assembly

1.027	1.031	1.039	1.049	1.059	1.067	1.064	1.064	1.068	STD FA
1.105	1.096	1.079	1.060	1.047	1.046	1.081	1.117	1.134	BP
2.438	2.317	2.099	1.831	1.567	1.345	1.224	1.146	1.106	CR
1.093	1.095	1.099	1.105	1.108	1.110	1.102	1.098	1.101	I-Tube
	1.037	1.050	1.067	1.081	1.103	1.085	1.084	1.102	
	1.081	1.055	1.023	1.004	0.979	1.057	1.122	1.162	
	2.183	1.940	1.642	1.367	1.107	1.054	0.992	0.912	
	1.099	1.108	1.120	1.127	1.142	1.117	1.112	1.129	
		1.074	1.111	1.125		1.121	1.119		
		1.006	0.935	0.923		1.020	1.142		
		1.643	1.262	1.012		0.786	0.753		
		1.128	1.159	1.164		1.142	1.133		
				1.140	1.138	1.109	1.105	1.126	
				0.931	0.983	1.082	1.155	1.200	
				0.771	0.676	0.718	0.697	0.619	
				1.167	1.152	1.110	1.097	1.113	
				1.127	1.138	1.111	1.109	1.129	
				1.030	1.113	1.153	1.195	1.232	
				0.708	0.608	0.639	0.625	0.564	
				1.137	1.129	1.084	1.066	1.078	
						1.133	1.131		
						1.223	1.250		
						0.537	0.533		
						1.068	1.039		
						1.133	1.110	1.109	
						1.230	1.249	1.279	
						0.577	0.587	0.550	
						1.001	0.951	0.937	
							1.109	1.130	
							1.262	1.291	
							0.631	0.646	
							0.855	0.769	

Guide Tube
Instrument Tube

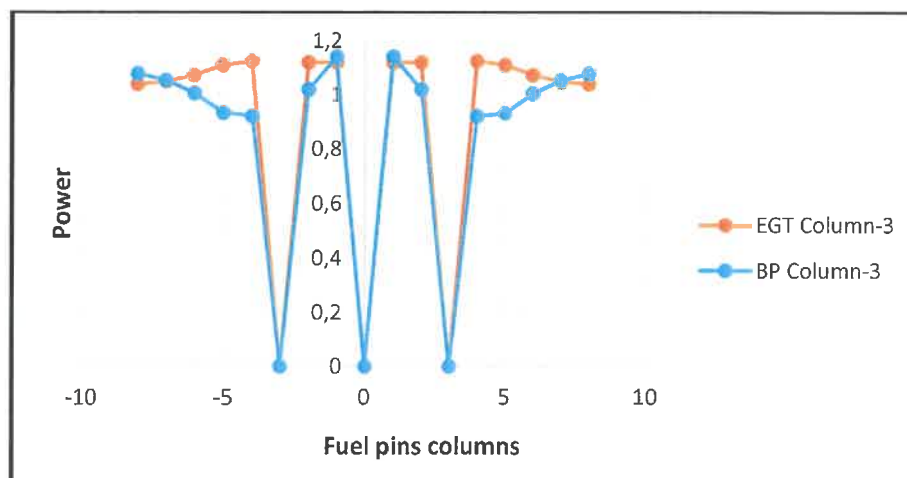


Figure 5-11: Power profiles for empty GT versus burnable poison

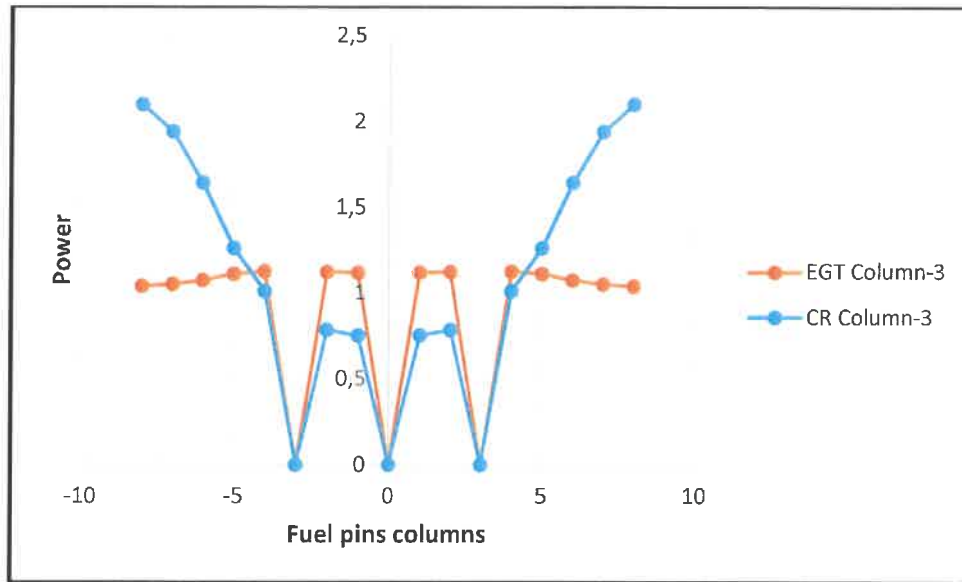


Figure 5-12: Power profiles for control rods versus empty GT

In Figure 5-12 it can be seen that the difference in the power profiles are much more pronounced than for the case with the burnable poison. This is as expected as the control rods are expected to shut down the reactor whereas the burnable poison are expected to reduce reactivity in the fuel at the beginning of cycle.

It can be concluded that inserting control rods in the fuel assembly reduced the power in the pins near the control rods but causes the power to increase in the pins that are away from the control rods. It can also be concluded that inserting the instrumentation tube in the fuel assembly reduced the power in the pins near the centre of the fuel assembly but causes the power to increase in the pins that are away from the centre of the fuel assembly.

As expected, we can see from comparing Figure 5-11 and Figure 5-12, that burnable poisons only mildly affect power profiles, although significantly alter reactivity. Control rods, on the other hand, dramatically impact all quantities in assemblies where they are present. This is consistent with their respective design goal, and explains why PWRs generally operate with control rods extracted, while using poisons and borated water for reactivity control.

CHAPTER 6 CONCLUSIONS AND RECOMMENDATIONS

This chapter provides the conclusions that have been reached during the study. It also offers recommendations for future studies.

6.1 Conclusion

The study was divided into four (4) main sections as follows:

- a. Preparation of the input models;
- b. Burn-up (HEADE against Serpent);
- c. Fuel assembly with spacer grid;
- d. Changing fuel enrichment (1.6 %, 2.4 % and 3.1 %); and
- e. Fuel assembly with control rods, fuel assembly with burnable poison pins and fuel assembly with an instrumentation pin.

The input models were prepared in both codes (HEADE and Serpent) according to the benchmark specifications. The author succeeded in converting the given 10 x 19 model to a model that correctly represented the BEAVRS 17 x 17 fuel assembly. This is evidenced in the fact that the k_{inf} and other parameters behaved as expected in both the material study and the enrichment study giving confidence that the models were prepared correctly. The results obtained when running the models lead to a conclusion that both codes were capable of handling the materials and geometry specifications.

When considering the burn-up which was investigated in Section 5.1, it was noted that the results obtained from the HEADE code were largely in good agreement with those obtained from the Serpent code with some differences here and there. This was evidenced by the small difference of about 399 pcm in the k_{inf} at BOL conditions obtained from the HEADE and the Serpent results, which is about 0.34 %. This could be attributed to the difference of the HEADE multi-group calculation with that of the continuous energy Monte-Carlo method used in Serpent.

It was further noted in Section 5.2 that HEADE produced expected results when the behaviour of ^{135}Xe and ^{149}Sm were considered. The curves produced by HEADE show that

the calculation performed were correct. This leads to a conclusion that HEADE calculates the burn-up parameters correctly.

The results regarding the inclusion of the spacer grid in the fuel assembly did not show the expected behaviour. When no change in reactivity was expected, a change of about 60 pcm was observed, and when a decrease in reactivity was expected, an increase of about 100 pcm was observed. A possible reason for this could be the numerical effects introduced when changing the number of computational grids in the model which was enabled by splitting the moderator volume (an annulus) into two concentric annuli. This unexpected behaviour however requires further investigation since the spacer grids are required components of the fuel assembly.

When considering the fuel assemblies with varying fuel enrichment as it was investigated in Section 5.4, it was noted that the k_{inf} values for fuel assemblies changed with an increase in fuel enrichment. It can be determined that the study shows the behaviour as was expected leading to a conclusion that HEADE produced acceptable results.

In Section 5.5 of this dissertation, the effect of the control rods, burnable poison and the instrumentation tube were investigated. It was noted that the insertion of the control rods in the fuel assembly decreases the reactivity. The BP, CR and IP studies showed behaviour as expected when applying the various changes to the HEADE model. However, further consideration to the self-shielding of these elements must still be considered.

A general conclusion can be reached from this study that the HEADE code may be viable for use in calculations regarding PWR power plants. It must be noted that some studies as listed below have to be undertaken before it can be concluded with certainty that the code can be used for power reactor calculations.

6.2 Recommendations for Future Studies

- A. It was seen that there were instances where the two codes differed by a large percentage. This cannot be ignored but it must be investigated. The instances referred to are:

1. Diffusion coefficient when HEADE is compared with Serpent, especially in the thermal energy group; and
 2. Absorption cross-section and fission cross-section in the fast energy group.
- B. The effect of the spacer grid needs to be investigated further since the differences observed of between 50 to 100 pcm could be considered as not negligible.

The comparative study between HEADE and Serpent has shown reasonable adequacy from HEADE, but some areas of concern remain. It would be preferable at this stage to rather use Serpent to calculate the group constants until the questions arising from this work have been resolved.

Further, as the differences cannot be ignored, it is also suggested that a further study to compare HEADE with some multi-group lattice physics codes such as NEWT in SCALE 6.2.1 should be carried out.

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APPENDIX A: MATERIAL DEFINITION OF MATERIALS USED IN THE MODELS

<i>Material Definition</i>				
<i>Material Number</i>	<i>Material Name</i>	<i>Material Number used in HEADE</i>	<i>User Definition using BEAVRS Data</i>	
1	Not used			
2	Borated Water	5 User Def	B-10	8.0042E-06
			B-11	3.2218E-04
			B	1.6509E-04
			H-1	4.9457E-02
			H-2	7.4196E-06
			H	4.9464E-02
			O-16	2.4672E-02
			O-17	9.3982E-06
			O-18	5.0701E-05
			O	2.4732E-02
3	Zircalloy-4	4 User Def	O-16	3.0743E-04
			O-17	1.1711E-07
			O-18	6.3176E-07
			O	3.0818E-04
			Cr-50	3.2962E-06
			Cr-52	6.3564E-05
			Cr-53	7.2076E-06
			Cr-54	1.7941E-06
			Cr	7.6852E-05
			Fe-54	8.6699E-06
			Fe-56	1.3610E-04
			Fe-57	3.1431E-06
			Fe-58	4.1829E-07
			Fe	1.4833E-04
			Zr-90	2.1827E-02
			Zr-91	4.7600E-03
			Zr-92	7.2758E-08
			Zr-94	7.3734E-03

<i>Material Definition</i>				
<i>Material Number</i>	<i>Material Name</i>	<i>Material Number used in HEADE</i>	<i>User Definition using BEAVRS Data</i>	
			Zr-96	1.1879E-03
			Zr	3.5148E-02
			Sn-112	4.6735E-06
			Sn-114	3.1799E-06
			Sn-115	1.6381E-06
			Sn-116	7.0055E-05
			Sn-117	3.7003E-05
			Sn-118	1.1669E-04
			Sn-119	4.1387E-05
			Sn-120	1.5697E-04
			Sn-122	2.2308E-05
			Sn-124	2.7897E-05
			Sn	4.8180E-04
4	UO ₂ (1.6 %)	1 User Def	U-234	3.0131E-06
			U-235	3.7503E-04
			U-238	2.2625E-02
			O-16	4.5895E-02
			O-17	1.7482E-05
			O-18	9.4313E-05
			O	4.6007E-02
4	UO ₂ (2.4 %)	1 User Def	U-234	4.4842E-06
			U-235	5.5814E-04
			U-238	2.2407E-02
			O-16	4.5828E-02
			O-17	1.7457E-05
			O-18	9.4176E-05
			O	4.5940E-02
4	UO ₂ (3.1 %)	1 User Def	U-234	5.7987E-06
			U-235	7.2175E-04
			U-238	2.2253E-02
			O-16	4.5850E-02
			O-17	1.7466E-05
			O-18	9.4222E-05

Material Definition				
Material Number	Material Name	Material Number used in HEADE	User Definition using BEAVRS Data	
			O	4.5962E-02
5	Helium	6 User Def	He-4	2.4044E-04
6	Stainless Steel 304	7 User Def	Si-28	9.5274E-04
			Si-29	4.8400E-05
			Si-30	3.1943E-05
			Si	1.0331E-03
			Cr-50	7.6778E-04
			Cr-52	1.4806E-02
			Cr-53	1.6789E-03
			Cr-54	4.1791E-04
			Cr	1.7671E-02
			Mn-55	1.7604E-03
			Fe-54	3.4620E-03
			Fe-56	5.4345E-02
			Fe-57	1.2551E-03
			Fe-58	1.6703E-04
			Fe	5.9229E-02
			Ni-58	5.6089E-03
			Ni-60	2.1605E-03
			Ni-61	9.3917E-05
			Ni-62	2.9945E-04
			Ni-64	7.6261E-05
			Ni	8.2390E-03
7		7 User Def	Ag-107	2.3523E-02
			Ag-109	2.1854E-02
			In-113	3.4291E-04
			In-115	7.6504E-03
			In	7.9933E-03
			Cd-106	3.4019E-05
			Cd-108	2.4221E-05
			Cd-110	3.3991E-04

Material Definition				
Material Number	Material Name	Material Number used in HEADE	User Definition using BEAVRS Data	
			Cd-111	3.4835E-04
			Cd-112	6.5669E-04
			Cd-113	3.3257E-04
			Cd-114	7.8188E-04
			Cd-116	2.0384E-04
			Cd	2.7215E-03
8	Borosilicate Glass	2 User Def	B-10	9.6506E-04
			B-11	3.9189E-03
			O-16	4.6511E-02
			O-17	1.7717E-05
			O-18	9.5581E-05
			O	4.6634E-02
			Al-27	1.7352E-03
			Si-28	1.6924E-02
			Si-29	8.5977E-04
			Si-30	5.6743E-04
			Si	1.8351E-02

APPENDIX B: BURN-UP RESULTS (HEADS).

Time (days)	Burn-up (MWD/tU)	k_{inf}	U-235 (atoms/cm ³)	U-238 (atoms/cm ³)	U-239 (atoms/cm ³)	Sm-149 (atoms/cm ³)	Xe-135 (atoms/cm ³)	Pu-238 (atoms/cm ³)	Pu-239 (atoms/cm ³)	Pu-240 (atoms/cm ³)	Pu-241 (atoms/cm ³)	Pu-242 (atoms/cm ³)
0	0	1.00818	1.14171E-04	6.88777E-03	3.04432E-20	3.04432E-20	3.04432E-20	3.04432E-20	3.04432E-20	3.04432E-20	3.04432E-20	3.04432E-20
0.25	10.417	0.99675	1.14086E-04	6.88771E-03	1.95821E-09	3.11529E-11	5.36918E-10	4.11133E-19	1.95821E-09	3.79763E-12	2.57562E-15	3.51095E-19
0.75	31.25	0.98355	1.13914E-04	6.88759E-03	1.68344E-08	2.51960E-10	1.15507E-09	3.10712E-17	1.68344E-08	3.96626E-11	7.88956E-14	2.70019E-17
1.5	62.499	0.97815	1.13658E-04	6.88741E-03	6.29453E-08	8.61079E-10	1.36724E-09	4.95200E-16	6.29453E-08	1.88555E-10	7.34949E-13	4.91815E-16
2.59	107.915	0.97587	1.13287E-04	6.88714E-03	1.70542E-07	2.05470E-09	1.40224E-09	4.34180E-15	1.70542E-07	6.73156E-10	4.44728E-12	5.06087E-15
12.95	539.576	0.97032	1.09812E-04	6.88460E-03	2.06072E-06	9.21688E-09	1.40966E-09	2.22547E-12	2.06072E-06	2.92956E-08	9.61497E-10	5.45379E-12
25.91	1079.568	0.96918	1.05643E-04	6.88143E-03	4.61982E-06	1.01828E-08	1.42528E-09	2.82835E-11	4.61982E-06	1.29349E-07	8.72557E-09	1.01734E-10
38.86	1619.144	0.96722	1.01663E-04	6.87825E-03	6.97345E-06	1.04659E-08	1.43822E-09	1.16764E-10	6.97345E-06	2.88518E-07	2.94185E-08	5.26145E-10
51.81	2158.719	0.96434	9.78530E-05	6.87507E-03	9.13342E-06	1.07299E-08	1.44854E-09	3.08195E-10	9.13342E-06	4.94321E-07	6.68275E-08	1.62569E-09
64.77	2698.712	0.96079	9.41971E-05	6.87187E-03	1.11219E-05	1.09836E-08	1.45681E-09	6.40974E-10	1.11219E-05	7.37208E-07	1.22880E-07	3.80629E-09
77.72	3238.287	0.95678	9.06896E-05	6.86866E-03	1.29535E-05	1.12232E-08	1.46338E-09	1.14951E-09	1.29535E-05	1.00925E-06	1.97987E-07	7.48733E-09
90.67	3777.863	0.95246	8.73183E-05	6.86544E-03	1.46450E-05	1.14481E-08	1.46854E-09	1.86581E-09	1.46450E-05	1.30474E-06	2.91756E-07	1.30859E-08
103.63	4317.855	0.94793	8.40725E-05	6.86220E-03	1.62105E-05	1.16590E-08	1.47249E-09	2.81969E-09	1.62105E-05	1.61927E-06	4.03261E-07	2.10023E-08
116.58	4857.431	0.94327	8.09503E-05	6.85894E-03	1.76589E-05	1.18565E-08	1.47541E-09	4.03601E-09	1.76589E-05	1.94864E-06	5.30958E-07	3.15858E-08
129.53	5397.007	0.93853	7.79428E-05	6.85567E-03	1.90014E-05	1.20420E-08	1.47745E-09	5.53932E-09	1.90014E-05	2.29007E-06	6.73386E-07	4.51665E-08
142.49	5936.999	0.93375	7.50423E-05	6.85238E-03	2.02478E-05	1.22163E-08	1.47871E-09	7.35271E-09	2.02478E-05	2.64132E-06	8.29064E-07	6.20450E-08
155.44	6476.575	0.92897	7.22483E-05	6.84907E-03	2.14040E-05	1.23801E-08	1.47930E-09	9.49283E-09	2.14040E-05	2.99978E-06	9.96150E-07	8.24439E-08
168.39	7016.151	0.92419	6.95538E-05	6.84575E-03	2.24779E-05	1.25343E-08	1.47931E-09	1.19784E-08	2.24779E-05	3.36393E-06	1.17322E-06	1.06586E-07
181.35	7556.143	0.91943	6.69528E-05	6.84241E-03	2.34768E-05	1.26798E-08	1.47880E-09	1.48271E-08	2.34768E-05	3.73255E-06	1.35896E-06	1.34672E-07
194.3	8095.719	0.91471	6.44454E-05	6.83905E-03	2.44048E-05	1.28168E-08	1.47784E-09	1.80481E-08	2.44048E-05	4.10374E-06	1.55171E-06	1.66802E-07
207.25	8635.294	0.91003	6.20260E-05	6.83567E-03	2.52679E-05	1.29461E-08	1.47648E-09	2.16555E-08	2.52679E-05	4.47665E-06	1.75036E-06	2.03110E-07
220.21	9175.287	0.90539	5.96896E-05	6.83227E-03	2.60716E-05	1.30882E-08	1.47477E-09	2.56624E-08	2.60716E-05	4.85055E-06	1.95392E-06	2.43717E-07
233.16	9714.862	0.90080	5.74365E-05	6.82886E-03	2.68189E-05	1.31834E-08	1.47276E-09	3.00714E-08	2.68189E-05	5.22396E-06	2.16099E-06	2.88621E-07

Time (days)	Burn-up (MWD/tU)	k_{inf}	U-235 (atoms/cm ³)	U-238 (atoms/cm ³)	U-239 (atoms/cm ³)	Sm-149 (atoms/cm ³)	Xe-135 (atoms/cm ³)	Pu-238 (atoms/cm ³)	Pu-239 (atoms/cm ³)	Pu-240 (atoms/cm ³)	Pu-241 (atoms/cm ³)	Pu-242 (atoms/cm ³)
246.11	10254.438	0.89626	5.52621E-05	6.82542E-03	2.75145E-05	1.32923E-08	1.47048E-09	3.48923E-08	2.75145E-05	5.59639E-06	2.37080E-06	3.37890E-07
259.07	10794.43	0.89177	5.31619E-05	6.82197E-03	2.81627E-05	1.33953E-08	1.46797E-09	4.01347E-08	2.81627E-05	5.96741E-06	2.58263E-06	3.91586E-07
272.02	11334.006	0.88735	5.11368E-05	6.81850E-03	2.87658E-05	1.34926E-08	1.46527E-09	4.57948E-08	2.87658E-05	6.33581E-06	2.79538E-06	4.49625E-07
284.97	11873.582	0.88298	4.91824E-05	6.81502E-03	2.93274E-05	1.35847E-08	1.46241E-09	5.18792E-08	2.93274E-05	6.70133E-06	3.00851E-06	5.12029E-07
297.93	12413.574	0.87867	4.72952E-05	6.81151E-03	2.98510E-05	1.36720E-08	1.45940E-09	5.83945E-08	2.98510E-05	7.06372E-06	3.22156E-06	5.78819E-07
310.88	12953.15	0.87442	4.54756E-05	6.80799E-03	3.03383E-05	1.37546E-08	1.45628E-09	6.5313E-08	3.03383E-05	7.42198E-06	3.43364E-06	6.49844E-07
323.83	13492.725	0.87024	4.37201E-05	6.80444E-03	3.07924E-05	1.38329E-08	1.45307E-09	7.26940E-08	3.07924E-05	7.77599E-06	3.64442E-06	7.25097E-07
336.79	14032.718	0.86611	4.20253E-05	6.80088E-03	3.12157E-05	1.39072E-08	1.44978E-09	8.04873E-08	3.12157E-05	8.12565E-06	3.85362E-06	8.04571E-07
349.74	14572.293	0.86206	4.03920E-05	6.79731E-03	3.16100E-05	1.39777E-08	1.44645E-09	8.86967E-08	3.16100E-05	8.47011E-06	4.06054E-06	8.88064E-07
362.69	15111.869	0.85807	3.88168E-05	6.79371E-03	3.19775E-05	1.40446E-08	1.44307E-09	9.73245E-08	3.19775E-05	8.80937E-06	4.26499E-06	9.75549E-07
375.65	15651.861	0.85414	3.72967E-05	6.79010E-03	3.23203E-05	1.41084E-08	1.43968E-09	1.06373E-07	3.23203E-05	9.14342E-06	4.46684E-06	1.06700E-06
388.6	16191.437	0.85028	3.58324E-05	6.78648E-03	3.26397E-05	1.41690E-08	1.43629E-09	1.15824E-07	3.26397E-05	9.47155E-06	4.66552E-06	1.16218E-06
453.37	18890.149	0.83244	2.92714E-05	6.76815E-03	3.38914E-05	1.44278E-08	1.41931E-09	1.68921E-07	3.38914E-05	1.09600E-05	5.66322E-06	1.69329E-06
518.14	21588.861	0.81603	2.38364E-05	6.74944E-03	3.47849E-05	1.46412E-08	1.40377E-09	2.31050E-07	3.47849E-05	1.23016E-05	6.52557E-06	2.30568E-06
582.9	24287.156	0.80120	1.93562E-05	6.73039E-03	3.54331E-05	1.48154E-08	1.39005E-09	3.00770E-07	3.54331E-05	1.34946E-05	7.26575E-06	2.97991E-06
647.67	26985.867	0.78796	1.56801E-05	6.71102E-03	3.59118E-05	1.49655E-08	1.37867E-09	3.76461E-07	3.59118E-05	1.45439E-05	7.89848E-06	3.69896E-06
712.44	29684.579	0.77626	1.26785E-05	6.69139E-03	3.62744E-05	1.51021E-08	1.36984E-09	4.56390E-07	3.62744E-05	1.54583E-05	8.43791E-06	4.44769E-06
777.2	32382.874	0.76601	1.02381E-05	6.67154E-03	3.65583E-05	1.52328E-08	1.36353E-09	5.38858E-07	3.65583E-05	1.62495E-05	8.89736E-06	5.21322E-06
841.97	35081.586	0.75705	8.26057E-06	6.65150E-03	3.67889E-05	1.53625E-08	1.35955E-09	6.22316E-07	3.67889E-05	1.69305E-05	9.28912E-06	5.98521E-06
906.74	37780.298	0.74926	6.66292E-06	6.63133E-03	3.69834E-05	1.54942E-08	1.35764E-09	7.05353E-07	3.69834E-05	1.75144E-05	9.62373E-06	6.75499E-06
971.5	40478.593	0.74249	5.37519E-06	6.61104E-03	3.71529E-05	1.56296E-08	1.35749E-09	7.86757E-07	3.71529E-05	1.80136E-05	9.91033E-06	7.51571E-06
1036.27	43177.305	0.73660	4.33851E-06	6.59067E-03	3.73044E-05	1.57693E-08	1.35879E-09	8.65566E-07	3.73044E-05	1.84400E-05	1.01568E-05	8.26244E-06

APPENDIX C: HEADE V/S SERPENT RESULTS

<i>Time</i>	<i>Burn-up</i>		<i>k_{inf}</i>		<i>Rel Err</i>	<i>Difference</i>	<i>Mass of U-235</i>		<i>U-235 Mass Difference</i>
<i>(Days)</i>	<i>MWD/tU</i>	<i>MWD/kgU</i>			<i>(%)</i>	<i>(pcm)</i>	<i>(kg)</i>	<i>(kg)</i>	<i>(%)</i>
	<i>HEADE</i>	<i>Serpent</i>	<i>HEADE</i>	<i>Serpent</i>			<i>HEADE</i>	<i>Serpent</i>	
0	0	0.000	1.00818	1.01155	7.90E-05	-337.82	6.83E+03	6.83E+03	0.00
0.25	10.417	0.010	0.99675	1.00015	8.90E-05	-341.44	6.82E+03	6.82E+03	0.00
0.75	31.25	0.031	0.98355	0.98676	8.10E-05	-321.92	6.81E+03	6.81E+03	0.00
1.5	62.499	0.062	0.97815	0.98131	7.60E-05	-317.09	6.80E+03	6.80E+03	0.00
2.59	107.915	0.108	0.97587	0.97891	8.20E-05	-305.41	6.78E+03	6.78E+03	0.00
12.95	539.576	0.540	0.97032	0.97262	7.80E-05	-230.21	6.57E+03	6.57E+03	0.02
25.91	1079.568	1.080	0.96918	0.97098	8.10E-05	-180.68	6.32E+03	6.32E+03	0.05
38.86	1619.144	1.619	0.96722	0.96856	7.50E-05	-134.09	6.08E+03	6.08E+03	0.09
51.81	2158.719	2.159	0.96434	0.96535	8.30E-05	-100.81	5.85E+03	5.84E+03	0.15
64.77	2698.712	2.699	0.96079	0.96148	8.20E-05	-68.84	5.63E+03	5.62E+03	0.21
77.72	3238.287	3.238	0.95678	0.95741	7.70E-05	-62.49	5.42E+03	5.41E+03	0.28
90.67	3777.863	3.778	0.95246	0.95273	7.80E-05	-27.04	5.22E+03	5.20E+03	0.36
103.63	4317.855	4.318	0.94793	0.94821	8.00E-05	-28.90	5.03E+03	5.01E+03	0.45
116.58	4857.431	4.857	0.94327	0.94309	8.30E-05	17.41	4.84E+03	4.82E+03	0.54
129.53	5397.007	5.397	0.93853	0.93808	8.40E-05	45.10	4.66E+03	4.63E+03	0.64
142.49	5936.999	5.937	0.93375	0.93316	8.50E-05	59.56	4.49E+03	4.46E+03	0.75
155.44	6476.575	6.477	0.92897	0.92797	8.50E-05	100.10	4.32E+03	4.28E+03	0.86
168.39	7016.151	7.016	0.92419	0.92310	8.30E-05	109.11	4.16E+03	4.12E+03	0.98
181.35	7556.143	7.556	0.91943	0.91810	8.40E-05	133.05	4.01E+03	3.96E+03	1.11
194.3	8095.719	8.096	0.91471	0.91304	8.30E-05	166.84	3.86E+03	3.81E+03	1.24
207.25	8635.294	8.635	0.91003	0.90799	8.70E-05	203.39	3.71E+03	3.66E+03	1.38
220.21	9175.287	9.175	0.90539	0.90309	8.60E-05	228.73	3.57E+03	3.52E+03	1.53
233.16	9714.862	9.715	0.90080	0.89816	8.00E-05	262.47	3.44E+03	3.38E+03	1.68
246.11	10254.438	10.254	0.89626	0.89315	8.90E-05	310.06	3.31E+03	3.25E+03	1.84
259.07	10794.43	10.794	0.89177	0.88861	8.60E-05	315.05	3.18E+03	3.12E+03	2.00
272.02	11334.006	11.334	0.88735	0.88399	8.60E-05	334.95	3.06E+03	2.99E+03	2.17
284.97	11873.582	11.874	0.88298	0.87908	9.00E-05	388.01	2.94E+03	2.87E+03	2.34
297.93	12413.574	12.414	0.87867	0.87475	9.20E-05	390.04	2.83E+03	2.76E+03	2.52
310.88	12953.15	12.953	0.87442	0.87012	8.90E-05	427.92	2.72E+03	2.65E+03	2.70
323.83	13492.725	13.493	0.87024	0.86576	9.20E-05	445.05	2.62E+03	2.54E+03	2.89
336.79	14032.718	14.033	0.86611	0.86139	9.30E-05	469.97	2.51E+03	2.44E+03	3.09
349.74	14572.293	14.572	0.86206	0.85686	9.60E-05	516.66	2.42E+03	2.34E+03	3.29
362.69	15111.869	15.112	0.85807	0.85282	9.40E-05	521.86	2.32E+03	2.24E+03	3.49
375.65	15651.861	15.652	0.85414	0.84844	9.10E-05	566.20	2.23E+03	2.15E+03	3.70
388.6	16191.437	16.192	0.85028	0.84467	9.70E-05	557.47	2.14E+03	2.06E+03	3.91
453.37	18890.149	18.890	0.83244	0.82560	9.40E-05	678.86	1.75E+03	1.67E+03	5.04
518.14	21588.861	21.589	0.81603	0.80842	9.80E-05	754.26	1.43E+03	1.34E+03	6.26
582.9	24287.156	24.287	0.80120	0.79320	9.60E-05	792.00	1.16E+03	1.08E+03	7.54
647.67	26985.867	26.986	0.78796	0.77997	1.10E-04	791.60	9.38E+02	8.62E+02	8.87
712.44	29684.579	29.685	0.77626	0.76828	9.60E-05	790.27	7.58E+02	6.88E+02	10.22
777.2	32382.874	32.383	0.76601	0.75833	9.70E-05	760.24	6.12E+02	5.49E+02	11.58
841.97	35081.586	35.082	0.75705	0.74988	9.90E-05	711.02	4.94E+02	4.38E+02	12.92
906.74	37780.298	37.780	0.74926	0.74249	0.0001	671.02	3.99E+02	3.49E+02	14.24
971.5	40478.593	40.479	0.74249	0.73620	0.0001	623.65	3.22E+02	2.78E+02	15.52
1036.27	43177.305	43.177	0.73660	0.73083	0.0001	572.16	2.60E+02	2.22E+02	16.76