

Uncertainty analysis of the fuel compact of the prismatic high temperature gas- cooled reactor test problem using SCALE6.1

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Declaration

I declare that the work I am submitting for assessment contains no section copied in whole or in part from any other source unless explicitly identified in quotation marks and with detailed, complete and accurate referencing.

Signed: _____

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Abstract

The IAEA CRP UAM on HTGRs has established international activities grouped into phases for the evaluation of HTGRs through sensitivity and uncertainty assessments. The assessments range from Reactor physics, Thermal-hydraulics and Depletion calculations. This study focuses on Reactor physics calculations and deals with calculations performed on the fuel pin cell model of the MHTGR-350 MW reference reactor design. The calculations were performed using the KENO-VI and TSUNAMI-3D codes, which are part of the SCALE 6.1 code package. The KENO-VI calculates the criticality of the pin cell, while TSUNAMI-3D uses solutions obtained from forward and adjoint calculations to provide additional sensitivity and uncertainty information.

The Reactivity-equivalent physical transformation RPT methodology was used to solve for the double-heterogeneity effect, which is an issue presented by HTGR concepts. Both the standard and modified RPT methods were investigated. It was found that the modified RPT model provides a much closer representation of double-heterogeneous model in terms of the neutron flux distribution compared on base-value calculations. The infinite multiplication factor for the homogeneous MHTGR-350 KENO-VI model underestimates the corresponding double-heterogeneous case in all temperature states. In all TSUNAMI-3D models of the fuel pin cell, it was found that the main contributor to the uncertainty in infinite multiplication factor was the capture of neutrons by the ^{238}U nuclei to release a gamma ray.

The computational results obtained in this study were compared with the existent body of literature.

Keywords: Uncertainty and sensitivity analysis, Modular High Temperature Gas-cooled Reactor, KENO-VI, TSUNAMI-3D, Reactivity-equivalent Physical Transformation, cross-section covariance data, infinite multiplication factor, sensitivity coefficients, SCALE 6.1

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Abbreviations

1D	one-dimensional
2D	two-dimensional
3D	three-dimensional
CRP	Coordinated Research Project
CDF	Cumulative Distribution Function
CE	Continuous Energy
CSAS	Criticality Safety Analysis Sequence with KENO-VI
CZP	Cold Zero Power
DOE	Department of Energy
ENDF	Evaluated Nuclear Data File
GeeWiz	Graphically Enhanced Editing Wizard
HFP	Hot Full Power
HTGR	High Temperature Gas-cooled Reactor
IAEA	International Atomic Energy Agency
IEA	International Energy Agency
IRP	Integrated Resource Plan
MCNP	Monte-Carlo N-Particle
MG	Multigroup Energy
MHTGR	Modular High Temperature Gas-cooled Reactor
MW	Mega Watt
NEA	Nuclear Energy Agency
NRC	Nuclear Regulatory Commission
OECD	Organization for Economic Co-operation and Development
ORNL	Oak Ridge National Laboratory
PDF	Probability Distribution Function
PSID	Preliminary Safety Information Document
RPT	Reactivity-equivalent Physical Transformation
SAMS	Sensitivity Analysis Module for SCALE
SCALE	Standardized Computer Analyses for Licensing Evaluation
SiC	Silicon Carbide
TRISO	Triple Coated Isotropic Particle
TSUNAMI	Tools for Sensitivity and Uncertainty Analysis Methodology Implementation
TWG-GCR	Technical Working Group on Gas-Cooled Reactors
UAM	Uncertainty Analysis in best-estimate Modelling
UCO	Uranium Carbide Oxide

CHAPTER 1 – INTRODUCTION

1.1 Background and overview

Over the years, surveys have been conducted on the world's dependency and usage of different energy sources. Energy sources include coal, oil, natural gas, nuclear, hydro etc. A publication was done by the International Energy Agency (IEA) regarding the world total primary energy supply and Figure 1 shows the statistics that have been collected over the years (IEA, 2014). It can be seen in the figure that the use for nuclear energy as a primary source has increased by more than five times in percentage terms between the years 1973 and 2012, following other sources of energy. Thus nuclear energy has increased in demand and plays a major part as a primary energy source. Nuclear energy has many applications including military (for nuclear weapons), nuclear medicine, electricity generation and production of isotopes for food preservation and increased agricultural production (Waltar, 2003).

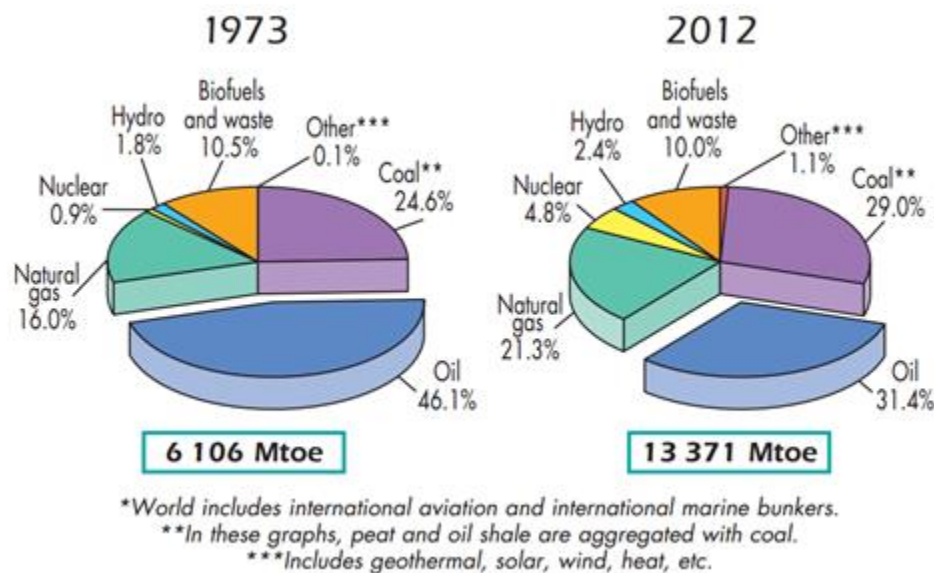


Figure 1 - Total primary energy supply by fuel

Source: (IEA, 2014).

The South African government has devised a plan to build new nuclear power plants that would deliver a total of 9600 MW of electricity to the national grid by the year 2030. This nuclear build programme is guided by the Department of Energy of South Africa and full updated documentation is available in the Integrated Resource Plan for Electricity 2010 - 2030 (DOE, 2013). To facilitate the process for the new build programme, research at the North West University (Potchefstroom Campus) within the School of Mechanical and Nuclear Engineering department is being conducted, focusing on various nuclear technologies. This study focuses on

the sensitivity and uncertainty analysis of the MHTGR-350 MW reactor design, particularly the fuel pin cell.

1.2 History of the MHTGR-350 reactor design

The High Temperature Gas-cooled Reactors (HTGRs) are generation 4-type reactor designs that have been developed since the 1950s. The design of the modular HTGR (MHTGR) began in the 1980s by HTGR designers working for INTERATOM a German company that adopted a pebble bed design (Idaho National Laboratory, 2011). This design was such that decay heat could be removed passively without the need for emergency core cooling. The geometric configuration of the MHTGR was such that the height of the core is three times larger than its diameter and this helps with the removal of decay heat radially and also passively from the uninsulated reactor vessel. The design of the MHTGR was intended for applications in electricity generation, the process heat and steam generation, and district heating. In the United States, a proposal was made by the year 1984 to the HTGR industry for a further development of the MHTGR that was much simpler, safer, facilitates economic growth and its power output could be sufficiently increased. To meet these requirements while also staying within the safety margins, a decision was reached to adopt an annular core design.

The first the annular core reactor design was the MHTGR-200 MW. The MHTGR-200 MW power output was found to be less economically competitive and an upgraded design was done by the Department of Energy and General Atomics to increase the power rating to 350 MW, resulting in the MHTGR-350 reactor design. Procedures were followed for the operation and licensing of MHTGR-350 and this included interventions with the NRC and the supply of the Preliminary Safety Information Document (PSID).

1.3 The role of IAEA CRP on HTGR UAM

Today the HTGRs are continually being developed and assessed on their safety and design features. Part of this work requires the use of accurate models and relevant computer codes for assessment of these features. With the increasing advances in simulation and modelling techniques, uncertainty studies in HTGRs are of importance, especially when calculating essential parameters such as the criticality or multiplication factor of the reactor system, the neutron flux and reactivity. Safety in the operation of nuclear reactors is of the highest priority, during both normal operation (steady state) and transient conditions. For a nuclear reactor to be licensed, it must be thoroughly inspected to confirm compliance with certain acceptance criteria called the regulatory limits. A few of the parameters that are considered to characterize safety of reactor operations include: maximum fuel temperature during loss of coolant accidents, loss of

offsite power, withdrawal of all control rods and main helium blower shutdown without any counter effects (Idaho National Laboratory, 2011).

The analysis tools of the HTGRs are currently being assessed with sensitivity and uncertainty analysis techniques. These analysis methods are today broadly employed in safety studies and are gradually being recognized and accepted by the regulating authorities (Reitsma, Strydom, Tyobeka, & Ivanov, 2012). In uncertainty analysis, calculations of the likelihood or probability that certain reactor parameters will stay within the imposed regulatory limits are performed at transient and steady state reactor operations. Sensitivity analysis investigates the effect of the input parameters (which may be burnable poison concentration, pellet density etc.) on the reactor behaviour (multiplication factor, conversion rate ratio etc.). The values of these inputs are varied within their upper and lower limits. The inputs that have the greatest influence on output parameters are assessed with sensitivity analysis and are ranked according to the sensitivity coefficients so as to find the spread in the output parameters of interest. Variations in their value may be due to methods and modelling approximations, nuclear data uncertainties, and assembly/fuel manufacturing uncertainties.

The International Atomic Energy Agency's (IAEA) Technical Working Group on Gas-Cooled Reactors (TWG-GCR) proposed a Coordinated Research Program (CRP) on HTGRs for Uncertainty Analysis in Modelling (UAM) with applications on Reactor physics, Thermal-hydraulics and Depletion calculations (Reitsma, Strydom, Tyobeka, & Ivanov, 2012). The benchmark problems have been defined for two reference reactor designs including the prismatic MHTGR-350 MW and the 250 MW Pebble Bed design. The objective of the IAEA CRP on HTGR UAM is to address uncertainty in the HTGR calculations through all these applications, which range from nuclear data, engineering uncertainties, and the methodology and uncertainties due computational codes used. The scope is divided into four phases and within each phase are pre-defined exercises to be performed. The IAEA CRP on HTGR UAM utilizes a community of the experts in different fields and from different countries to allow comparison and assessment of sensitivity and uncertainty analyses in these applications and to provide recommendations for further development of these analyses methods.

In this study, the uncertainty and sensitivity analysis is performed using benchmark specification of the IAEA's MHTGR-350 MW reactor core, particularly the fuel pin cell. It is involved in the Phase I: Exercise I:1a and Exercise I:1b as part of the international activity exercise which focuses on the neutronics calculation. Only a steady state operation is considered and not transient incidents which are beyond the scope of this study. The KENO-VI criticality calculation code, together with its sensitivity and uncertainty assessment code, TSUNAMI-3D, are used to carry out this study. All these codes are embedded in the SCALE 6.1 code package

(Oak Ridge National Laboratory, 2011), which has various other codes called the modules necessary for criticality, shielding and depletion analysis of reactor systems and can work together to perform calculations (as a sequence), or can run a simulation individually (stand-alone).

1.4 Neutronic analysis codes

In this study, the MHTGR-350 fuel pin cell model is developed in KENO-VI code together with its uncertainty model using the assessment code TSUNAMI-3D. Various neutronic analysis codes exist that could have been used to model the fuel pin and these include HELIOS (Cho, Joo, Cho, & Zee, 2002), MCNP6 (Goorley, et al., 2015), and SERPENT (Leppänen, 2010). The SCALE 6.1 code system however was chosen as it is capable of propagating the uncertainty information of the cross-section directly from nuclear data libraries for reactor systems. Other codes would require separate pre-processors of the cross-sections for uncertainty propagation.

1.5 The concept of uncertainty and its sources

The models that are used in the scientific world serve to represent real systems, capturing important processes occurring in a complex system. For model input parameters that have greatest influence on reactor behaviour or output, their contribution to the uncertainty is a major concern and thus needs to be investigated. The investigation of uncertainties arising from these parameters is needed to address issues relating to design and safety operation of a nuclear reactor. In an attempt to model nuclear reactor behaviour, there are sources of uncertainties that have an influence in the reactor's response parameters (such as the calculated reaction rate, power density and reactivity) and these can cause the response parameters to deviate from their designed or optimum values. These uncertainty inputs arise from the following aspects (Oberkampf, DeLand, Rutherford, Diegert, & Alvin, 2001):

- Model form: Scientific models serve to approximate real physical systems and the quality of this approximation reflects levels of insight into the system. By modelling the fuel pin cell and its components in a block, for instance, the extent to which the model representation deviates from the observed system structure induces the uncertainty.
- Input parameters: Parameters that are input to the models are first measured or evaluated by pre-processor models, and this introduces the uncertainty in a parameter. Certain reactor output parameters (i.e. power) are dependent on input parameter values (i.e. fuel concentration) and the input uncertainties should be taken into account by error propagation.

- Methodological uncertainties: The uncertainties are associated with the numerical methods and modelling approximations on how well they are represented on a code. For example, KENO-VI used in this study uses a set of quadratic equations to build geometrical shapes (Hollenbach, 2011) of the fuel pin cell of the MHTGR-350 reference reactor design.
- Manufacturing uncertainties: The deviation of unit cell dimensions or densities of nuclides in a system from their optimum design values can cause the output parameters of interest to also deviate from their safety margins. Their tolerance limits should be considered.

For this study, only the uncertainties associated with input parameters from the nuclear data libraries are investigated. The approximations such as energy group condensation and assembly homogenization in a single assembly environment are only investigated in the next lattice physics calculation exercise and not in this study.

1.6 Problem statement

The uncertainty treatments in the Light Water Reactors (LWRs) have already been established through international collaborative activities. Significant progress has been documented in the OECD/NEA Light Water Reactor Uncertainty Analysis in best-estimate Modelling benchmark activity (Ivanov, et al., 2013). Since there are not enough literature studies on the uncertainty propagation in the HTGRs to assess on the design and safety features, the IAEA CRP proposed a development of the methodology for best-estimate plus uncertainty and sensitivity analysis of the HTGR through Reactor physics, Thermal hydraulics and Depletion applications and this is divided into four phases (Reitsma, Strydom, Tyobeka, & Ivanov, 2012).

This study deals with an isolated benchmark activity focused on Reactor physics applications (Phase 1) where the uncertainties of the response parameter (effective multiplication factor) are propagated and the sensitivities of other nuclear parameters of importance are calculated for a fuel pin cell model of the reference reactor design MHTGR-350 MWt. The uncertainty response parameter is propagated from the nuclear data library ENDF-B-VII.0. The SCALE 6.1 code package is utilized for the calculations.

1.7 Aims of the study

The aims of this study are to:

- Install SCALE 6.1 code successfully.
- Build input models and optimize the parameters of the model.
- Build the uncertainty models.
- Investigate the impact of cross-section uncertainties on the MHTGR-350 fuel pin cell, and relate the findings to the published work for LWR and HTGR design types.
- Quantify the accuracy of the standard and modified RPT approaches in SCALE 6.1.
- Determine the main contributors to resulting uncertainties in the reactivity for the pin cell.

1.8 Dissertation layout

The following layout has been adopted for the dissertation:

CHAPTER 2 – General theory and literature survey

The benchmark specifications followed in this study for the analysis of MHTGR-350 reactor design are presented in this chapter. The general theory and supporting literature study on the uncertainty and sensitivity treatment are outlined in this chapter, together with the techniques or methods used for the uncertainty and sensitivity analysis.

CHAPTER 3 – Specific theory

The theory that is most applicable to this study pertaining sensitivity and uncertainty analysis is outlined. The fundamental equations and their computational forms for code implementation to produce sensitivity and uncertainty parameters are also covered in this chapter.

CHAPTER 4 – Methodology and study approach

The steps which were followed to build MHTGR-350 models in KENO-VI and TSUNAMI-3D codes are presented in this chapter.

CHAPTER 5 – Results and discussions

The nominal or base-value results together with uncertainty assessment results obtained from KENO-VI and TSUNAMI-3D models are presented in this chapter. Confirmation for convergence of results and optimization parameters used in the models are outlined. Discussions thereof are also provided.

CHAPTER 6 – Conclusions and future recommendations

This chapter presents the concluding remarks drawn from assessment of results obtained and problems experienced while conducting this study. Recommendations for future work are provided.

CHAPTER 2 – GENERAL THEORY AND LITERATURE SURVEY

2.1 Introduction

In this chapter, the IAEA CRP on HTGR UAM benchmark specifications of the reference MHTGR-350 MW reactor design are presented. Since this study is mainly focused on the fuel pin cell of the MHTGR-350 MW reactor design, its specifications are further presented for use in model development, simulation and the evaluation process. Previously conducted studies that are in line with this study, the comparisons thereof and the relevance with regard to this study are also presented.

2.2 An overview of the IAEA CRP on MHTGR-350 MW reactor

The MHTGR-350 reactor design used in this study is a prismatic-type HTGR designed to provide a thermal output of 350 MW (Gougar H., 2012). The core is made of cylindrical, hexagonal fuel blocks which are surrounded by a ring of solid graphite hexagonal blocks. The graphite blocks are all of the same size and are replaceable. The replaceable graphite blocks are surrounded by a region of permanent reflector graphite blocks. Figure 2 shows the plan-view of the MHTGR-350 core layout and Figure 3 shows the corresponding axial-view.

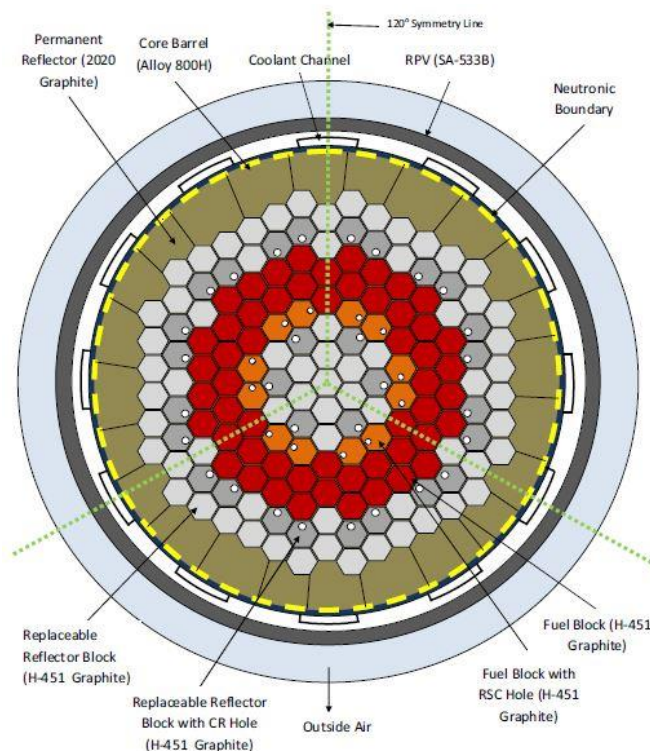


Figure 2 - Plan-view of the MHTGR-350 core layout.

Source: (Reitsma, Strydom, Tyobeka, & Ivanov, 2012)

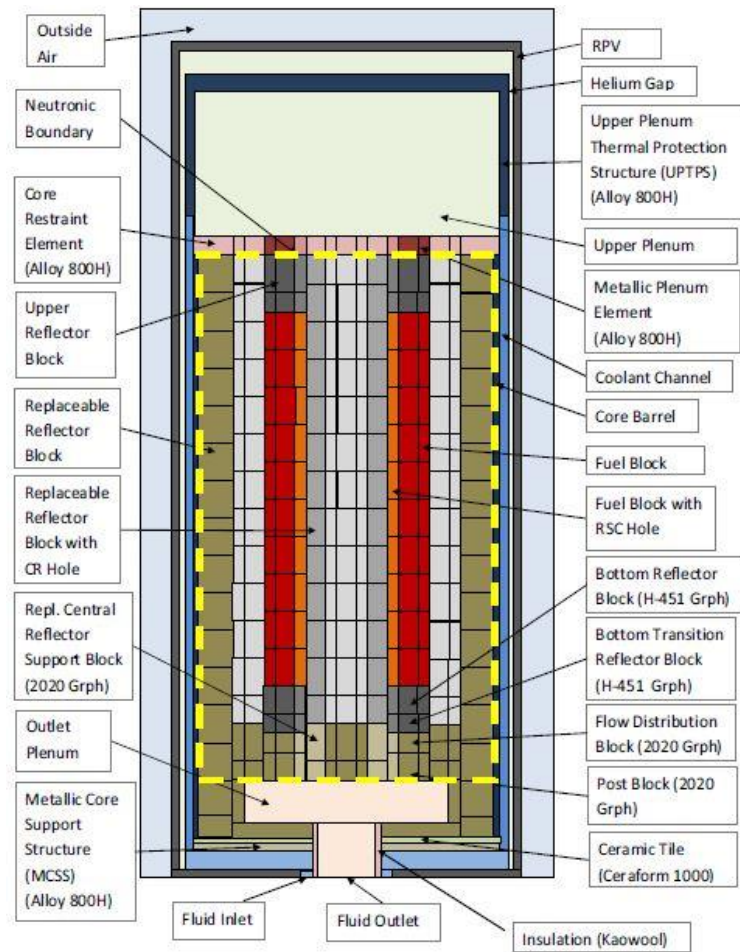


Figure 3 - Axial-view of the MHTGR-350 core layout
Source: (Reitsma, Strydom, Tyobeka, & Ivanov, 2012)

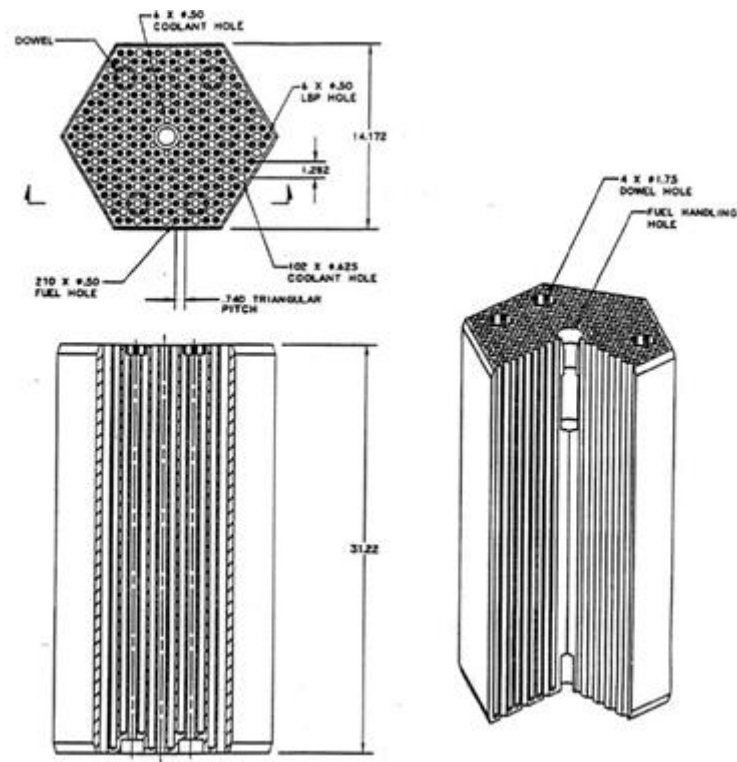


Figure 4 - Fuel block.

Source: (Reitsma, Strydom, Tyobeka, & Ivanov, 2012)

As can be seen in Figure 3, hexagonal fuel blocks are stacked vertically to form a column, which rests on support structures. Each column has ten blocks. A single fuel block is shown in Figure 4. The active core columns (which form a three-row annulus) have twelve channels for reserve shutdown material. The reflector columns that surround the three-row annulus have a total of 30 columns that have channels for control rods.

Table 1 below summarizes the major design and operating conditions of the IAEA's MHTGR-350 reference reactor design (Gougar H., 2012).

Table 1 - Design specifications and operating characteristics of the MHTGR-350.

MHTGR Characteristic	Value
Installed thermal capacity	350 MW(t)
Installed electrical capacity	165 MW(e)
Core configuration	Annular
Fuel	Prismatic Hex-Block fuelled with Uranium Oxycarbide fuel compact of 15.5 wt% enriched ^{235}U (average)
Primary coolant	Helium
Primary coolant pressure	6.39 MPa
Moderator	Graphite

Core outlet temperature	687 °C
Core inlet temperature	259 °C
Mass Flow Rate	157.1 kg/s
Reactor Vessel Height	22 m
Reactor Vessel Outside Diameter	6.8 m

2.3 Description of the MHTGR-350 fuel pin cell

The IAEA CRP MHTGR-350 unit cell reference design is shown in Figure 5a below. The fuel pin cell is a hexagonal structure consisting of the fuel compact in the central region surrounded by the helium gap, and the latter is surrounded by the block graphite. Within the fuel compact are the TRISO particles dispersed in the graphite matrix. Figure 5b shows the corresponding MHTGR-350 fuel block. The manner in which the hexagonal fuel pin cell forms the lattice structure for the fuel block is shown. Note also that the helium channel and the burnable poison compacts also make up separate hexagonal units building up the lattice structure of the fuel block.

In this study, an assumption is made that this fuel pin cell is surrounded by pin cells of the same type across all its boundaries. This then means the use of reflective boundary conditions.

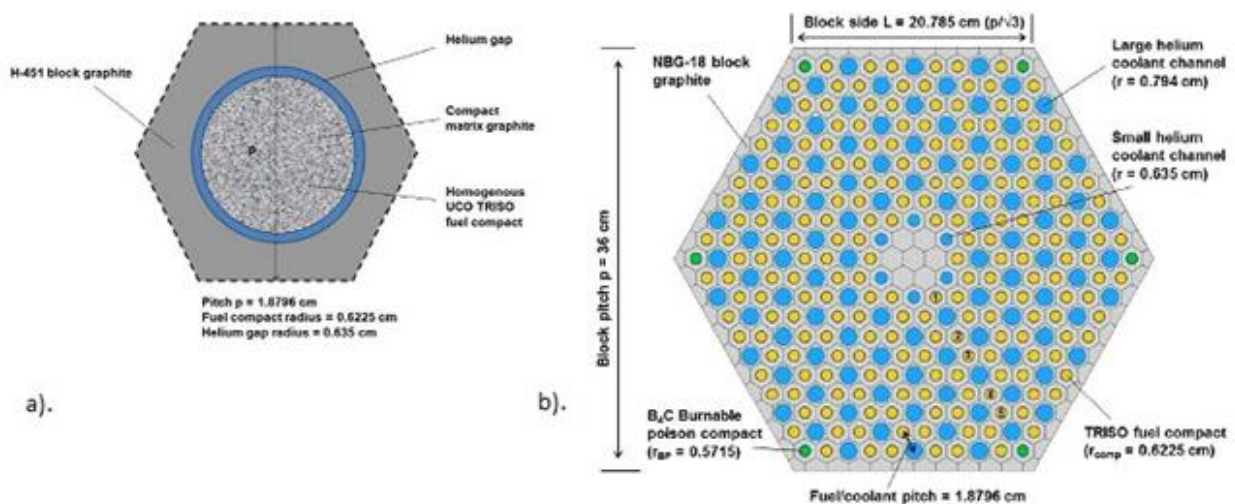


Figure 5 - The MHTGR-350 fuel pin cell and hexagonal block

Source: (Strydom G. B., 2015)

Two scenarios that are investigated on the pin cell are classified under Exercise I-1a and Exercise I-1b of the IAEA CRP Benchmark (Strydom & Bostelmann, Prismatic HTGR Benchmark Definition: Phase 1 INL/LTD-15-34868, June 2015). Exercise I-1a treats the central fuel region as a homogeneous mixture while Exercise I-1b specifies a double-heterogeneous mixture, where the fuel lumps (TRISO particles) are dispersed in a

moderating graphite matrix. The double-heterogeneous term in this case comes from the fact that TRISO particles have multiple coated layers of different material composition (constituting the first level of heterogeneity). The fuel pin cells together with the coolant pin cells form a hexagonal lattice in the fuel assembly and this constitutes the second level of heterogeneity. The coolant pin cells have the same geometry as the fuel pin cells, however the compacts in the fuel pin cells are replaced by coolant channels. In the benchmark specification, the coolant channels are specified with either the small or large radii (0.635 or 0.794 cm respectively).

Figure 6 shows the structure of the heterogeneous TRISO particle.

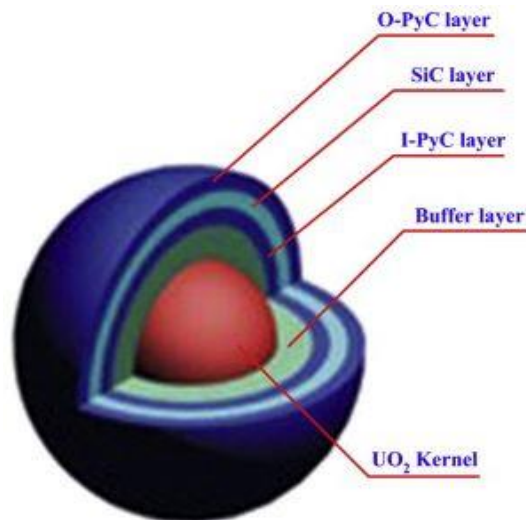


Figure 6 - Structure of the TRISO fuel particle.

Source: (Yang, et al., 2013).

In each scenario, the Cold Zero Power (CZP) at temperature 293 K and Hot Full Power (HFP) at temperature 1200 K reactor conditions are imposed to investigate their resonance self-shielding effects on the multigroup parameters of interest. The following tables highlight the operating conditions, dimensions and material compositions of the fuel pin cell (Strydom G. B., 2015).

Table 2 - Operating conditions.

Parameter/Reactor condition	CZP	HFP
Temperature of all material in fuel compact [K]	293	1200
Temperature of helium in gap [K]	293	1200
Temperature of H-451 block graphite [K]	293	1200
Reactor power [MWt]	0.3500	350

Table 3 - Dimensions for the homogeneous model.

Parameter	Dimension [cm]
Fuel compact outer radius	0.6225
Fuel/helium gap outer radius	0.6350
Unit cell pitch	0.9398
Fuel compact height	4.9280

Table 4 - Dimensions for the double-heterogeneous model.

Parameter		Dimension [cm]
TRISO fuel particle	UCO kernel radius	2.125E – 02
	Porous carbon buffer layer outer radius	3.125E – 02
	Inner PyC outer radius	3.525E – 02
	SiC outer radius	3.875E – 02
	Outer PyC outer radius	4.275E – 02
Average TRISO Packing Fraction		0.3500 [dimensionless]
Fuel compact outer radius		0.6225
Fuel/helium gap outer radius		0.6350
Large helium coolant channels radius		0.7940
Unit cell pitch		0.9398
Fuel compact height		4.9280

Table 5 - Number densities for the homogeneous model.

Nuclide		Number density [atoms/b·cm]
Homogenized fuel region	²³⁵ U	1.5765E – 04
	²³⁸ U	8.4864E – 04
	¹⁶ O	1.5094E – 03
	Graphite	6.9958E – 02
	²⁸ Si	2.8457E – 03
	²⁹ Si	1.4456E – 04
	³⁰ Si	9.5408E – 05
Coolant channel	⁴ He	2.4600E – 05
H-451 block graphite	Graphite	9.2756E – 02

Table 6 - Number densities for the double-heterogeneous model.

Number densities		Nuclide	Number density [atoms/b·cm]
TRISO fuel particle	Kernel	²³⁵ U	3.6676E – 03
		²³⁸ U	1.9742E – 02
		¹⁶ O	3.5114E – 02
		Graphite	1.1705E – 02
	Porous carbon	Graphite	5.2646E – 02
	iPyC	Graphite	9.5263E – 02
	SiC	²⁸ Si	4.4159E – 02
		²⁹ Si	2.2433E – 03
		³⁰ Si	1.4805E – 03
		Graphite	4.7883E – 02
	OPyC	Graphite	9.5263E – 02
Compact matrix		Graphite	7.2701E – 02
Coolant channels		⁴ He	2.4600E – 05
H-451 block graphite		Graphite	9.2800E – 02

These benchmark specifications of the IAEA CRP MHTGR-350 unit cell operating conditions, dimensions and material composition were used to construct and simulate the models in KENO-VI and TSUNAMI-3D codes. The benchmark specifications are also utilized to build the standard and modified RPT models of the pin cell. The methodologies followed to build such models are described in detail in Chapter 4.

2.4 Uncertainty and sensitivity analysis theories

Sensitivity analysis investigates a change in model output parameters due to variations of the model input parameter within a prescribed range (Loucks & van Beek, 2005). The objective for this analysis is to determine the input parameters that greatly influence the output parameters of importance. The input parameters that are associated with uncertainties are called uncertain input parameters.

In this study, the most strongly contributing input parameters to sensitivities of output parameters of importance are ranked using sensitivity coefficients. The input parameters are however only those associated with the nuclear parameters. The more comprehensive population of input parameters will be investigated in later studies. Sensitivity coefficients represent the percentage effect on a response or output parameter due to a percentage change of an input parameter. Mathematically, this is defined as the derivative of the output parameter with respect to a given input parameter (Loucks & van Beek, 2005). The generalized perturbation method described in Chapter 3 to follow outlines how the sensitivity coefficients are generated, which is the method adopted in this study.

Uncertainty analysis, on the other hand, measures a set of possible outcomes of model output parameters by varying the input parameters all at once. A probability of occurrence is then defined for each set of input parameters. The likelihood that a system parameter acquires a certain value is characterized by probability distribution functions, which follows in the next Section 2.5.

2.5 Probability distribution functions

Consider a given value of a system parameter which varies, and that its variation over space and time cannot be predicted with certainty. That is, one cannot exactly say what the value will be, but can ascribe a probability that the value will lie within a specified range. Then that parameter is called a random variable. Many types of probability distributions exist that are used to describe the probability of observing a selected range of values for a random variable.

If a random variable X can only have discrete sets of values, then its probability distribution can be described in a histogram (Figure 7a). The functions $P_X(X)$ and $f_X(X)$ ascribe probability to a random variable for having a specific value. For a random variable that can assume a continuous

set of real values, a continuous distribution is used to describe its probability distribution (Figure 7b). If all possible outcomes of values for the random variable are counted, then the sum of all probabilities must be equal to one. The probability that the value x of X will lie within range of values between u and v (i.e. the area bounded under the curve by u and v) is represented in Figure 7c.

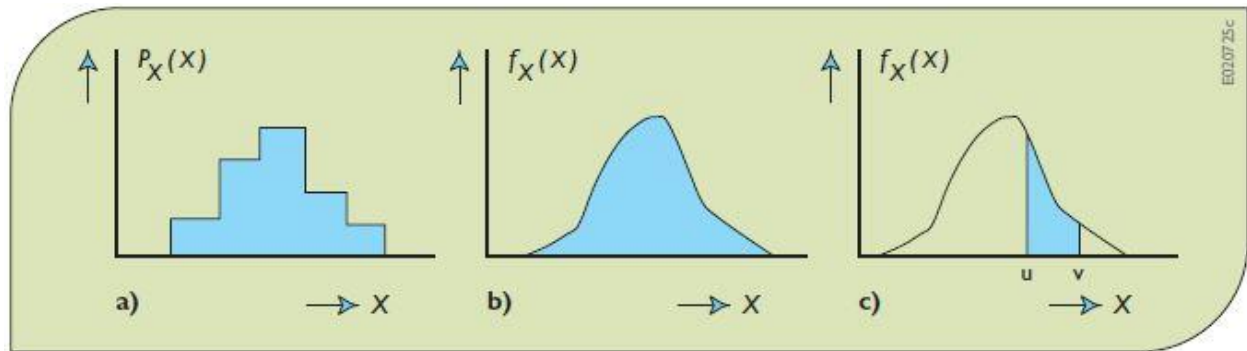


Figure 7 - Probability distributions of discrete and continuous random variable X .

Source: (Loucks & van Beek, 2005)

Complete uncertainty quantification is met only when all sources of uncertainties to probability distributions for each input and output variables in a model are identified, as was addressed under Section 1.5.

2.6 Propagation of uncertainties

A number of output parameters or variables exist which are dependent on certain input parameter values. For example, when the radius r of a sphere has been measured it can be used to find its volume V . This is found by using a simple relation:

$$V = \frac{4}{3}\pi r^3 \quad (1)$$

The input parameters that are associated with the errors induce the uncertainty of the output parameters which are expressed as functions based on them and the uncertainty or error is propagated (Taylor, 1997). Mathematical expressions can be derived that relates error propagation between input and output parameters. Given that the input variables have a dependency or are related to each other whose measured values are $a, b, c \dots x, y, z$ and the associated uncertainties $\delta a, \delta b, \delta c \dots \delta x, \delta y$ and δz , their effect on the output variable which is a function of these input variables can be determined. Let Q be the measured output variable from a function $f(x)$, as shown in Figure 8 below.

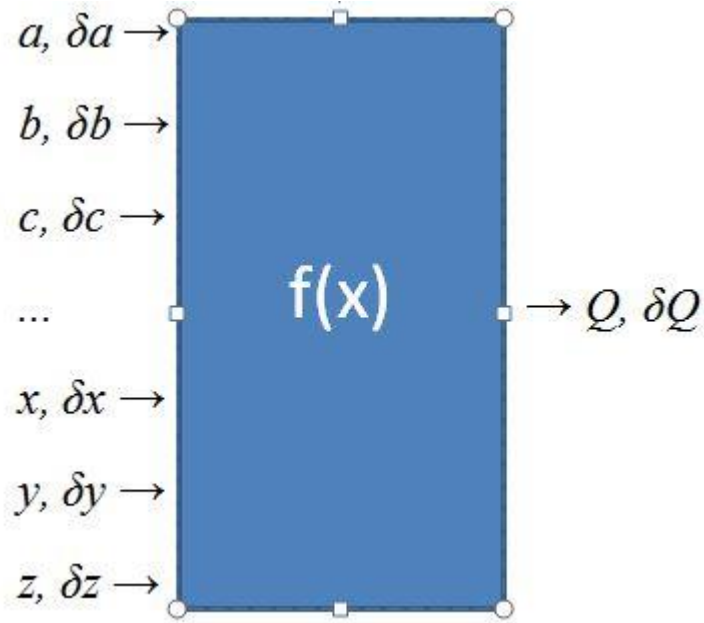


Figure 8 - Propagation of uncertainties.

Suppose that several values of a function $Q(x, y)$ which depends on x and y variables only are obtained by measuring pairs of such variables $(x_i, y_i) \dots (x_N, y_N)$ N times i.e. $Q_i = Q(x_i, y_i)$ for $i = 1, 2, \dots, N$. When the $x_1, x_2, \dots, x_N$ and $y_1, y_2, \dots, y_N$ values are all close to the mean values $\bar{x}$ and $\bar{y}$ respectively, the mean value of $Q(x, y)$ can be represented as follows:

$$\bar{Q} = \frac{1}{N} \sum_{i=1}^N Q_i = \frac{1}{N} \sum_{i=1}^N \left[Q(\bar{x}, \bar{y}) + \frac{\partial Q}{\partial x} (x_i - \bar{x}) + \frac{\partial Q}{\partial y} (y_i - \bar{y}) \right] \quad (2)$$

Covariance is a term from statistical and probability theory which is used to indicate the relation of two variables. The mathematical formula for covariance is shown below (Taylor, 1997):

$$COV(x, y) = \sigma_{xy} = \frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})(y_i - \bar{y}) \quad (3)$$

When the measurements of the x and y variables are independent, the covariance tends to approach zero. For any value of y_i , the $(x_i - \bar{x})$ term is equally likely to be positive or negative. This implies that after many measurements, the positive and negative terms in Equation (3) balances and the $1/N$ factor forces $COV(x, y)$ to be zero. When the measurements of the x and y variables are not independent, the covariance would not be zero and the product of $(x_i - \bar{x})$ and $(y_i - \bar{y})$ terms will be positive and thus $COV(x, y)$ will be positive. This holds for significantly large measurements.

Another parameter, called variance measures how far a set of numbers are distributed and is expressed when the variables are identical:

$$VAR(x) = COV(x, x) = \frac{1}{N} \sum_{i=1}^N (x_i - \bar{x})^2 \quad (4)$$

A statistical treatment in propagating the input uncertainties for calculating the uncertainty in the output parameter is adopted and uncertainties are expressed as standard deviations. The following Table 7 summarizes a manner in which the uncertainty in Q is propagated based on functions of real variables (Taylor, 1997).

Table 7 - Uncertainty propagation in basic mathematical expressions.

Function	Standard deviation (δQ)
$Q = x + \dots + z - (u + \dots + w)$	$\delta Q = \delta x + \dots + \delta z + \delta u + \dots + \delta w$
$Q = \frac{x \cdot y \cdot \dots \cdot z}{u \cdot v \cdot \dots \cdot w}$	$\frac{\delta Q}{ Q } \approx \frac{\delta x}{ x } + \frac{\delta y}{ y } + \dots + \frac{\delta z}{ z } + \frac{\delta u}{ u } + \frac{\delta v}{ v } \dots + \frac{\delta w}{ w }$
$Q = x^n$	$\frac{\delta Q}{ Q } = n \cdot \frac{\delta x}{ x }$

The use of uncertainty propagation in line with this study is to address the impact of the uncertainty information provided in the nuclear data library (ENDF-B-VII.0 used as input to KENO-VI and TSUNAMI-3D models) on the calculated output response parameter k_{inf} and other parameters of importance.

2.7 Literature study

The literature survey that is most applicable and related to the work at present was performed as these lay a foundation and a guide to how the objectives of the work can be fulfilled. A selected few of these papers are outlined below and each follows a consistent flow structure to make it possible to extract useful information that is delivered.

Six papers were selected which elaborate more on important key concepts faced with the MHTGR-350 pin cell, and these include the double-heterogeneity effects, uncertainties in multigroup cross-sections and the analysis codes used in their models. Concise paragraphs are provided towards the end of each paper highlighting on their relevance with the work at hand. The referenced work was combined for the upbringing of this paper, which will contribute to a wide development of methodology for uncertainty treatment in the design and safety analysis of the HTGR.

2.7.1 IAEA GT-MHTR benchmark calculations by using the HELIOS/MASTER physics analysis procedure and the MCNP Monte Carlo code (Lee, Kim, Cho, Noh, & Lee, 2008)

Purpose:

To validate the already existing physics analysis tools and the models for the GT-MHTR reactor.

Method:

The calculations were performed on the pin and block elements of the GT-MHTR reactor using the information provided by the IAEA GT-MHTR benchmark. The HELIOS/MASTER deterministic code and MCNP Monte Carlo code were used to perform the calculations. The 2-step procedure was applied to the HELIOS/MASTER code for the generation of few group constants through a transport lattice calculation.

The Reactivity-equivalent Physical Transformation method was applied to get rid of the double-heterogeneity effects that most deterministic codes cannot accurately model. The reflector cross-sections (where there is strong core-reflector interaction) were generated by application of the equivalence theory.

The results obtained with the HELIOS/MASTER code were compared with those of MCNP solutions which were used as a reference. It was observed that the maximum multiplication factor difference between these codes was about 693 pcm for pin cell calculations and about 457 pcm for fuel block calculations. The control rod worths found in both codes are consistent with the maximum difference found to be 3090 pcm. At core calculations level, the maximum difference in control rod worths found in the codes were reduced from 21500 pcm to 7700 pcm after the surface dependent discontinuity factors were considered.

Conclusion:

- The 2-step procedure of the HELIOS/MASTER code can be utilized as the standard analysis tool for prismatic VHTR.

This study focuses on a pin cell calculation that is similar to the one of the GT-MHTR reactor. Double-heterogeneity effects are also treated here by use of the RPT theory. The results of this study will be used when analysing the continuous energy and multigroup calculations. The methodology employed with the RPT method will also be compared when using the RPT method with KENO-VI.

The block calculations are required in the next Exercise I-2 of the IAEA CRP on HTGR and are not included in this work.

2.7.2 The IAEA Coordinated Research Program on HTGR Uncertainty Analysis: Phase I Status and Initial Results (Reitsma , Strydom, Bostelmann, & Ivanov, 2014)

Purpose:

To present an overview of the IAEA CRP current status and the first results for homogeneous and double-heterogeneous exercises of Phase I for the MHTGR-350 fuel pin cell.

Method:

Simulations were performed using SCALE/KENO-VI and Serpent Monte Carlo reactor criticality codes on the fuel pin cell of the MHTGR-350 reactor using the information provided by the IAEA CRP on HTGR benchmarks definition. The sensitivity and uncertainty quantification step is performed using SCALE/TSUNAMI module. Two exercises are defined: a homogeneously mixed fuel region, and a double-heterogeneous fuel region in the compact of the MHTGR-350 reactor at CZP and HFP states. Regular and random arrangements of TRISO particles were investigated within the double-heterogeneous exercise. For a fair comparison with KENO-VI code that can only establish a regular TRISO particle arrangement, the Serpent regular structure is used as a reference.

Solutions provided with Serpent using ENDF-B-VII.0 library at continuous energy mode were used as a reference as shown in Table 8 below:

Table 8 - Multiplication factor reference results obtained with Serpent.

Model	$k_{inf.} \pm \sigma$	
	CZP	HFP
Serpent (Homogeneous)	1.27827 ± 0.00013	1.20302 ± 0.00014
Serpent (Regular)	1.31906 ± 0.00012	1.24672 ± 0.00013

Comparisons with KENO-VI results also using ENDF-B-VII.0 library were made. The relative differences of KENO-VI and Serpent codes for the homogeneous model were at most 445 ± 25 pcm and 360 ± 27 pcm at CZP and HFP, respectively. The double-heterogeneous model in KENO-VI was built in regular TRISO particle arrangement and the differences with Serpent regular structure were 231 ± 3 pcm and 133 ± 3 pcm at CZP and HFP respectively.

Uncertainty assessment was performed on the homogeneous model. The top five nuclide reactions contributing to the uncertainty (given as relative standard deviation $\% \Delta k/k$) in the $k_{inf.}$ of the MHTGR-350 pin cell found to be $^{238}\text{U} (n, \gamma)$, $^{235}\text{U} (\bar{\nu})$, $^{235}\text{U} (n, \gamma)$, $^{238}\text{U} (n, n)$ and C-graphite (n, n) in order of increasing magnitude at CZP and HFP respectively. Sensitivity profiles for the nuclide reactions that impact significantly on a change in $k_{inf.}$ value were plotted as functions of incident neutron energy.

Conclusion:

- Good agreement of solutions provided with KENO-VI and Serpent Monte Carlo codes was observed.
- The neutron nuclide reactions contributing most to uncertainty in k_{inf} were found to be ^{238}U (n, γ) and ^{235}U ($\bar{\nu}$) covariance matrices.

In this study similar calculations on the MHTGR-350 fuel pin cell are performed using only the KENO-VI and TSUNAMI-3D modules of SCALE 6.1 code package. Revised benchmark specifications from the IAEA CRP for the pin cell are used.

2.7.3 Results for Phase I of the IAEA Coordinated Research Project on HTGR Uncertainties (Strydom, Bostelmann, & Yoon, INL/EXT-14-32944 Revision 2, 2015)**Purpose:**

To give an overview of the phases and exercises of the IAEA CRP on HTGR benchmark specifications. An update of the reference results for phase I is provided.

Method:

The Monte Carlo codes Serpent and KENO-VI were utilized for the simulation of the fuel pin cell and fuel block of the MHTGR-350 reactor, classified under Exercise I-1 and Exercise I-2 respectively of the IAEA CRP on HTGR updated benchmark definition. In Exercise I-1, the homogeneous and double-heterogeneous mixture of the fuel compact region is investigated. In Exercise I-2, three scenarios are investigated: a fresh fuel block, a depleted fuel block, and a fresh block surrounded by the graphite reflector and depleted fuel blocks (a super cell).

Convergence studies were performed in all the exercises prior to obtaining the infinite multiplication factors k_{inf} . The CZP and HFP conditions were analysed for the fuel pin cell and only the HFP state was analysed for the fuel blocks.

Serpent solutions were used as a reference for fuel pin cell and fuel block calculations. The obtained results were 1.25995 ± 0.00012 and 1.18462 ± 0.00014 at CZP and HFP respectively for the homogeneous model. The relative differences with KENO-VI models and Serpent solutions were at most 580 ± 20 pcm and 332 ± 20 pcm for CZP and HFP respectively. The double-heterogeneous Serpent solutions were 1.31865 ± 0.00012 and 1.24657 ± 0.00013 at CZP and HFP states respectively. The corresponding KENO-VI solutions had relative differences with Serpent results amounting at most to 753 ± 20 pcm and 1060 ± 20 pcm at CZP and HFP conditions respectively.

The k_{inf} values for fresh, depleted and fresh block surrounded by the graphite reflector and depleted fuel blocks, respectively, are 1.06304 ± 0.00008 , 0.96528 ± 0.00013 and 1.05010 ± 0.00005 obtained with Serpent. At most, the relative differences of these solutions with those obtained with KENO-VI were 934 ± 19 pcm, 853 ± 23 pcm and 669 ± 18 pcm.

Conclusion:

- The homogenization of the fuel compact underestimates the reference double-heterogeneous model k_{inf} in the order of several hundred pcm.
- The infinite multiplication factor obtained with KENO-VI continuous energy calculation exceeds those obtained with Serpent for the fuel block calculations excluding the super cell).
- KENO-VI multigroup calculation of k_{inf} underestimates equivalent results obtained with KENO-VI continuous energy calculation except for the super cell. Differences in these calculations decrease with increase in model size from a pin cell to a fuel block.

Only the fuel pin cell calculations are performed in this study. The results obtained can later be used for the next level in fuel block calculations.

2.7.4 Modeling Doubly Heterogeneous Systems in SCALE (Goluoglu & Williams, 2005)

Purpose:

To present the modelling capabilities of SCALE sequences in double-heterogeneous system and further test and evaluate them against MONK9 code results.

Method:

Capabilities have been added to the SCALE code system for modelling of double-heterogeneous systems using either CSAS or CSAS6 which are control modules that use Monte Carlo codes KENO V.a or KENO-VI functional modules for 3D analyses, respectively. Also, this capability has been added in TRITON control module that use NEWT functional module for 2D analyses.

The information provided by the OECD/NEA Nuclear Science Committee, Working Party on the Physics of Plutonium Fuels and Innovative Fuel Cycles were used to test the capabilities on two test problems. These were performed on UO_2 fuel pebbles that contain 0.091 cm outer diameter of TRISO particles enriched to 8.2% of uranium, and the PuO_2 fuel pebbles containing 0.066 cm outer diameter of TRISO particles. The plutonium weight percent/plutonium isotope for this test problem was defined as follows:

2.59/ ^{238}Pu , 53.85/ ^{239}Pu , 23.66/ ^{240}Pu , 13.13/ ^{241}Pu and 6.77/ ^{242}Pu .

The capability is utilized by specifying a unit cell type called DOUBLEHET in the input file, which allows specifications of the TRISO particle coating dimensions, the isotopic compositions and its volume fraction in graphite matrix. Running the simulation will execute CENTRM and PMC modules. The point-wise flux disadvantage factors in the coated particles are calculated. These are then used to generate cell weighted point wise cross-sections for homogenized fuel region. CENTRM uses the point wise cross-sections and calculates flux distribution in the fuel element, and these are used by PMC to calculate multigroup problem dependent cross-sections for the final analysis.

This study was performed using KENO V.a and KENO-VI MC codes, where double-heterogeneous results were compared with homogeneous treatment on UO_2 and PuO_2 fuel pebbles. KENO V.a showed percentage difference of about 0.08 between double-heterogeneous and homogenous treatment, and the difference was also about 0.08 in the respective KENO-VI calculation using infinite array of UO_2 fuelled pebbles. Similar assessments were done on the infinite array of PuO_2 fuelled pebbles and differences found were about 0.2 in both KENO V.a and KENO-VI. A comparison of these results with those obtained with MONK9 showed differences of about 0.007 for UO_2 fuelled pebbles, and differences of about 0.017 for PuO_2 fuelled pebbles.

Conclusion:

- Double-heterogeneous systems can be modelled with CSAS, CSAS6, and TRITON sequences of SCALE.
- In all cases, the results found with KENO V.a and KENO-VI modules were in excellent agreement as they both use the same resonance-shielded cross-sections.

In this study, the double-heterogeneous effects presented by the MHTGR-350 pin cell are analysed using CSAS6 control sequence of KENO-VI. The added DOUBLEHET cell capability is utilized within this control sequence.

2.7.5 Development and verification of the coupled 3D neutron kinetics/thermal-hydraulics code DYN3D-HTR for the simulation of transients in block-type HTGR (Rohde, et al., 2012)

Purpose:

To present the current status of the development of the DYN3D reactor dynamics code for applications in transient behaviour of the block-type HTGR. This development is based on the equivalent DYN3D code that is utilized for steady-state 3D and transient analysis of the LWRs.

Method:

One of the developments on the code includes its ability to generate the cross-section data while double-heterogeneous effects were considered. Both the standard and the modified RPT models are described in this paper although only the modified RPT model was investigated. To this end the modified RPT model was considered and verification was done by performing calculations on a prismatic block-type HTGR fuel lattice. For this, the 3D BGCore MCNP-based code was used to obtain reference results which were compared with those of the 2D BGCore and deterministic based HELIOS1.9 codes.

Plots of k_{inf} as a function of burnup and fuel temperature (600 K, 900 K and 1200 K) were obtained from 3D and 2D BGCore codes and the difference in results between the codes were between 0.1% and 0.15%. These plots were generated again for the 2D HELIOS 1.9 code. Comparison of 2D HELIOS 1.9 model with the 3D BGCore MCNP based code the differences were between 0.3% and 0.6%. These results indicated that the modified RPT methods can reproduce the neutron flux (which were normalized per lethargy width) of the reference double-heterogeneous model accurately and results are in good agreement.

Other developments included the implementation of the SP_3 neutron transport method into the DYN3D code in a multigroup mode. The reason for this was to get rid of the deficiency of the diffusion approximation as applied to systems that have core layouts which are highly heterogeneous. The 3D heat conduction module was developed and implemented in DYN3D for HTGR applications. The aim was to take into consideration the temperature reactivity feedback to neutronics and this has shown that the heat produced by conduction in the graphite blocks becomes well distributed.

Conclusion:

- The results obtained with RPT methods in BGCore and HELIOS 1.9 codes agree very well with the detailed geometry solutions.
- The DYN3D-HTR code needs further verification and validation. Verification at core level was performed with use of DYN3D results and comparing them with those of reference Monte Carlo solutions. Validation of the code is a currently a challenge due to the lack of experimental data.

In the present work, the standard and modified RPT homogenization techniques are applied to the MHTGR-350 fuel pin cell which presents double-heterogeneity effects. Although the standard RPT method was not investigated in the paper since it does not allow decoupling of temperatures of the fuel and compact graphite, it is adopted in the present study since all materials in the fuel

compact are assigned the same temperatures. The effects of fuel temperature at 293 K (CZP) and 1200 K (HFP) on the system's k_{inf} are investigated.

2.7.6 Acceleration of Monte Carlo Criticality Calculations Using Deterministic-Based Starting Sources (Ibrahim, Peplow, Wagner, Mosher, & Evans, 2011)

Purpose:

To evaluate the defaulted approach of defining the initial source distribution by using KENO-VI deterministic calculations for improving reliability and efficiency in Monte Carlo criticality calculations.

Method:

The two test problems provided by the OECD/NEA Expert Group on Source Convergence in Criticality Safety Analysis were utilized. These were the pin-cell array reflected with LWR spent fuel with more reactive and less reactive regions, and a 5x5x1 array of highly enriched uranium (HEU) metal spheres in the air.

On the pin-cell array, two scenarios were investigated: symmetric (Case 2_1) and asymmetric (Case 2_3) axial compositions. Three starting sources in all the scenarios were specified for the Monte Carlo calculations:

1. A uniform source in axial direction.
2. A starting source that is based on forward criticality calculation.
3. A starting source that is based on adjoint criticality calculation with the source fixed.

On the 5x5x1 array of HEU metal spheres, the above 2 and 3 starting sources for pin cell array were retained, with additional starting sources defined as follows:

1. A uniform source distributed among all spheres.
2. A nonuniform source, where more neutrons are concentrated in one of the spheres at the edges.

The reference multiplication factors for the two test problems were obtained using KENO-VI where large numbers of skipped and active cycles were specified. This was based on the use of Shannon entropy which indicates convergence of source distribution. The exact numbers of skipped and active cycles when the fission source converges were noted. Using these numbers, calculations of the new multiplication factors for the test problems were performed and their results obtained. These multiplication factors were restricted to fall within a standard deviation of $2E-4$ of the reference calculations. The times taken to complete these new calculations were recorded.

Lastly, the Monte Carlo starting sources (the skipped and starting sources) provided by KENO-VI code were used to calculate the multiplication factors of these test problems and their respective simulation run times were recorded.

With this information, the difference between multiplication factors between the reference and deterministic-based calculations was recorded as $\Delta \pm \sigma$. Another variable, called the speedup factor, was calculated and is defined as the ratio between time taken by Monte Carlo calculation with uniform starting source to fall in the required standard deviation of 2E-4 for the multiplication factor, and the total simulation time with other starting sources. The results are as follows:

Table 9 - Results obtained from the pin-cell test problem.

	$\Delta \pm \sigma$ [pcm]	Speed-up factor
Case 2_1		
Uniform	-10 ± 20	1
Forward	14 ± 20	1.6
Adjoint	3 ± 19	1.3
Case 2_3		
Uniform	14 ± 18	1
Forward	-3 ± 19	1.8
Adjoint	28 ± 17	1.1

Table 10 - Results obtained from the spheres test problem.

	$\Delta \pm \sigma$ [pcm]	Speed-up factor
Uniform	-58 ± 19	1
Non-uniform	63 ± 19	0.7
Forward	-7 ± 19	1.2
Adjoint	8 ± 18	0.6

Conclusion:

- The default approach adopted in Monte Carlo calculations for starting sources proved to speed up source convergence and increases efficiency in the simulations.
- This approach generated multiplication factor values very close to those of reference solutions in all test cases evaluated.
- The evaluation supports current activities to accelerate Monte Carlo reactor analyses with FW-CADIS method requiring forward deterministic calculation.
- Deterministic source distribution will be adopted in future work for starting source of Monte Carlo calculations.

The speedup factors are not a central focus in this study and should be recommended for future work. Convergence studies are performed in this study for quality assurance that results collected are accurate and under-sampling problems are prevented.

CHAPTER 3 – SPECIFIC THEORY

3.1 Introduction

In this chapter, the specific theory needed to conduct this research project pertaining sensitivity and uncertainty analysis with the aid of the SCALE 6.1 code package is outlined. A brief description of the SCALE 6.1 code package is provided together with the underlying KENO-VI and TSUNAMI-3D modules used to model and analyse the MHTGR-350 fuel pin cell.

3.2 Nuclear data libraries

Nuclear data serves to provide the measured probabilities of different types of reactions involving nuclei of the atoms. The data is used to provide input to models and simulations including fission reactor calculations, shielding and radiation protection calculations. For this study, it is used for criticality calculation of the MHTGR-350 pin cell model. The reaction types include scattering, fission, absorption etc. and probabilities that these different nuclear reaction types happen are characterized by the cross-sections, which are functions of energy and angle (Stacey, 2007).

Various organizations exist that periodically review the experimental nuclear data results and first ensure that measurement results are of high quality before they are made available to the public as a nuclear data library. A few of these organizations include (Stacey, 2007):

- The Joint Evaluated Fission and Fusion File organization (JEFF).
- Japanese Nuclear Data Committee that handles the Japanese Evaluated Nuclear Data Library (JENDL).
- The Cross-Section Evaluation Working Group which handles the ENDF-B file.
- The Russian Evaluated Nuclear data File (BROND).

Throughout this study, the ENDF-B-VII.0 file version is utilized for provision of nuclear data input to the fuel pin cell model of the MHTGR-350 reactor design used by the codes.

3.3 The Monte Carlo methods

The main goal in nuclear reactor theory is the determination of how the neutrons in a reactor system are distributed while taking into account the various types of interactions (scattering, absorption, fission etc.) it undergoes. Consideration of all these interactions in transport equations is a major challenge. The Monte Carlo method simulates the neutron transport by considering a series of the interactions a neutron undergoes, and using random numbers to present types of these interactions and their probabilities of occurrence along the neutron trajectory and all these

are added to characterize their entire behaviour in the reactor system. A Monte Carlo method uses a stochastic process to simulate the neutron transport.

A sequence of steps followed in Monte Carlo methods are described below (Stacey, 2007):

- The geometric dimensions of the system and the number densities of materials it contains are defined. The medium is treated as piecewise homogeneous.
- The source of neutrons which is predominantly fission has a distribution in space, energy and directions are characterized by probability and cumulative distribution functions (PDF and CDF). The definition for location in space, energy and direction (for two angular variables) for the neutron source is arrived at by generation of random numbers and selection of the CDF for each of these definitions.
- The neutron is allowed to move a certain distance until it experiences an interaction or leaks from the system. The distance that the neutron will move is defined by the choice of a random number.
- The types of nuclide that a neutron collides with and the resulting reaction type are determined in this step by generation of random numbers and selection of the PDF and CDF. For absorption reactions, the neutron life is terminated. For elastic or inelastic scattering reactions, the new interaction point and the neutron energy after scattering are obtained by random sampling.
- These processes are repeated until the neutrons leak from the medium or are being absorbed in the medium.

3.4 The Boltzmann transport equation

In nuclear reactor theory a focus is put on the determination of neutron distribution within a reactor system. Knowledge of such a distribution allows one to determine various reaction rates happening in the system and the analysis of the fission power in the reactor. For this the Boltzmann transport equation is used. The equation is derived by considering the neutron balance in an arbitrary volume element from where the reactions take place and is mathematically expressed as (Hollenbach, 2011):

$$\begin{aligned} \frac{1}{v} \frac{\partial \phi}{\partial t}(\vec{X}, E, \vec{\Omega}, t) + \vec{\Omega} \cdot \nabla \phi(\vec{X}, E, \vec{\Omega}, t) + \Sigma_t(\vec{X}, E, \vec{\Omega}, t) \phi(\vec{X}, E, \vec{\Omega}, t) \\ = S(\vec{X}, E, \vec{\Omega}, t) \\ + \int_{E'} \int_{\Omega'} \Sigma_s(\vec{X}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}, t) \phi(\vec{X}, E', \vec{\Omega}', t) d\vec{\Omega}' dE' \end{aligned} \quad (5)$$

The symbols used above have the following meanings:

$\phi(\vec{X}, E, \vec{\Omega}, t)$ = The neutron flux per unit energy at energy E along direction Ω at position X and time t.

$\Sigma_t(\vec{X}, E, \vec{\Omega}, t)$ = The total macroscopic cross-section of the medium at position X, energy E, direction Ω and time t.

$\Sigma_s(\vec{X}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}, t)$ = The macroscopic scattering cross-section per unit energy at position X for scattering of neutrons with initial energy E' and direction Ω' resulting in neutrons with E and direction Ω at time t.

$S(\vec{X}, E, \vec{\Omega}, t)$ = The neutron source born at position X with energy E, having direction Ω at a time t.

In this work, CENTRM functional module of SCALE 6.1 (to be described in Section 3.6) performs a 1D discrete ordinates calculation for the generation of the neutron flux using the deterministic approximations of Equation (5) assuming a lattice or reflected structure of the system being modelled i.e. the MHTGR-350 pin cell. These fluxes are then used by PMC as problem-dependent weight function for multigroup microscopic cross-section evaluation.

The next two sections describe the generation of the cross-section data which are required in the Boltzmann transport equation in multigroup energy calculations.

3.4.1 Cross-section generation in multigroup energy calculations

By using the flux as the weighting function, the multigroup cross-section is mathematically defined as (Williams & Hollenbach, 2011):

$$\sigma_{z,r,g}^j = \frac{\int_{\Delta E_g} \sigma_{z,r}^j(E) \phi_z(E) dE}{\int_{\Delta E_g} \phi_z(E) dE} = \frac{\int_{\Delta E_g} \sigma_{z,r}^j(E) \phi_z(E) dE}{\phi_{z,g}} \quad (6)$$

where:

$\phi_{z,g}$ = The multigroup flux is a particular zone

$\sigma_{z,r,g}^j$ = The zone-average group cross-section

ΔE_g = Discrete energy group interval

3.4.2 Cross-sections in continuous energy calculations

In continuous energy mode, the cross-section data is directly read from the nuclear data library. Thus there is no need to collapse the cross-section sets into groups as was described in Section 3.4.1.

3.5 Resonance cross-sections and the influence of temperature

It has been addressed in Section 3.2 that the nuclear data libraries provide us with the measured probabilities of different types of reactions involving nuclei of the atoms. The probability for a certain type of nuclear reaction to take place is expressed in terms of the cross-section σ . The units for cross-sections are area and are normally expressed as barn i.e. $1 \text{ barn} = 10^{-28} \text{ m}^2 = 10^{-24} \text{ cm}^2$. Figure 9 and Figure 10 below show the capture and fission cross-sections of ^{238}U and ^{235}U , respectively.

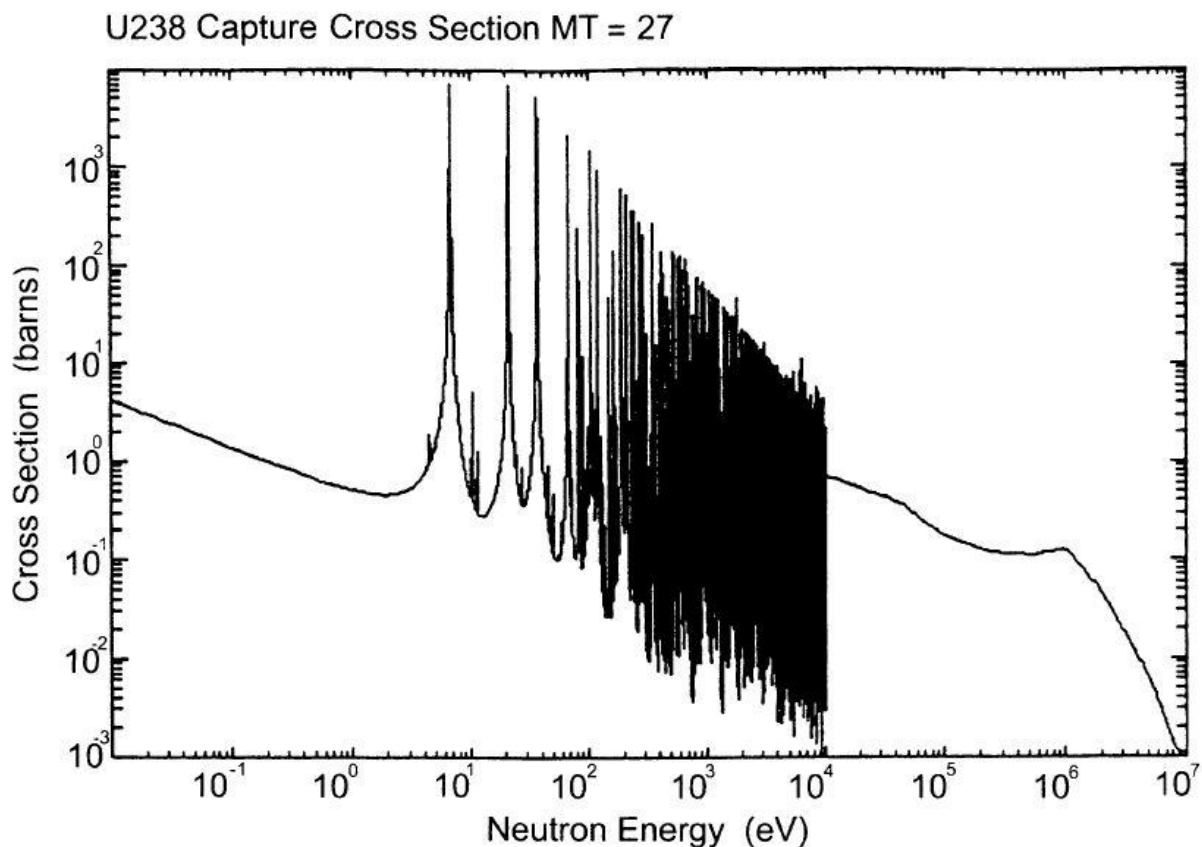


Figure 9 - The capture cross-section of U-238

Source: (Stacey, 2007)

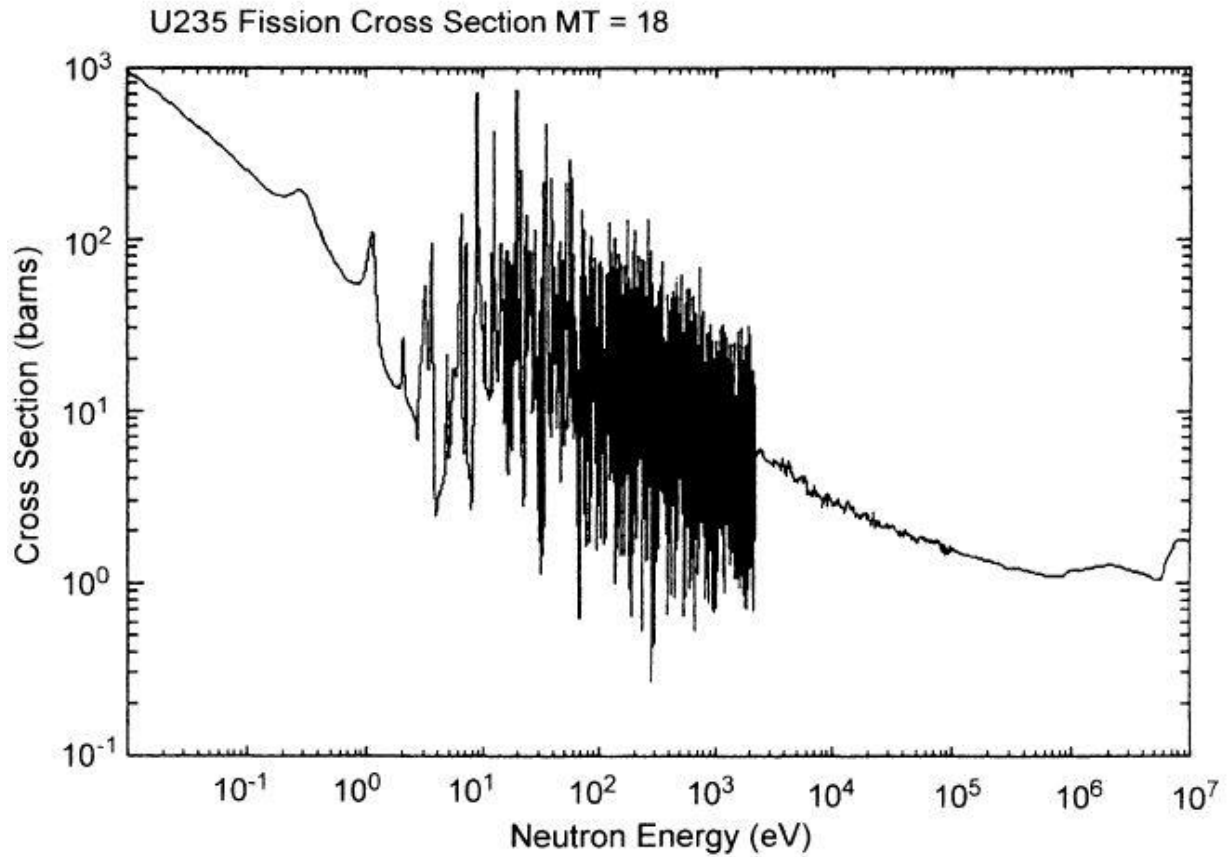


Figure 10 - The fission cross-section of U-235

Source: (Stacey, 2007)

The region between neutron energies of about $10^0 - 10^4$ eV in the figures above, where peaks in cross-sections occur, is called the resonance region. When an incident neutron is captured by the nucleus of an atom to form a compound nucleus, a certain amount of energy becomes available due to the binding energy. Additionally, there is thermal energy associated with the neutron. Let the sum of these energies be equal to E_{in} . The compound nucleus can exist in a number of excited states besides the ground state. Let E_{res} be the energy required to excite one such state from the lower state. When $E_{in} = E_{res}$, then the probability of neutron capture is large and thus the resonance condition will be achieved (Stacey, 2007).

The capture cross-section reactions averaged over the motion of the nucleus can be given by:

$$\sigma_Y(E, T) = \sigma_0 \frac{\Gamma_Y}{\Gamma} \left(\frac{E_0}{E} \right)^{\frac{1}{2}} \psi(\xi, x) \quad (7)$$

where:

$$\psi(\xi, x) = \frac{\xi}{2\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-1/4(x-y)^2\xi^2} \frac{dy}{1+y^2} \quad (8)$$

Equation (7) is known as the single level Breit-Wigner formula and Equation (8) is an integral over the relative motion of the neutron and nucleus. An assumption is made that nuclear motion can be described by the use of the Maxwellian distribution: T and E are the temperature and energy of the neutron in the lab system, $x = 2(E - E_0/\Gamma)$. The symbols used above mean the following:

σ_0 = Peak value of the cross-section.

E_0 = Neutron energy in the centre-of-mass at which σ_0 occurs.

Γ = The width of the resonance.

Γ_γ = Partial width for neutron capture.

Γ_f = Partial width for fission.

The parameter ξ characterizes the nuclear motion according to the equation:

$$\xi = \frac{\Gamma}{(4E_0kT/A)^{1/2}} \quad (9)$$

A in the above is the atomic mass in [amu] and k is the Boltzmann constant [eV/K]. Figure 11 below illustrates the dependence of the ψ function on the temperature T. When the temperature is increased, the peak value of ψ at E_0 decreases and the function also broadens. This phenomenon depicted in Figure 11 is called Doppler resonance broadening (Stacey, 2007).

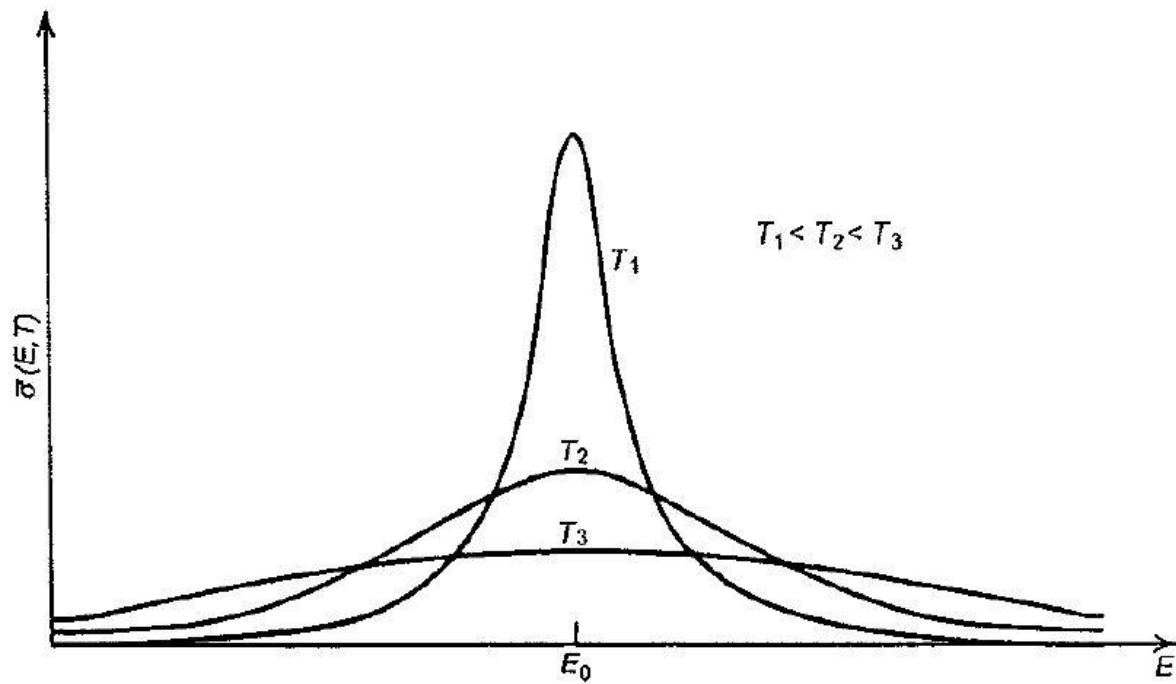


Figure 11 - Broadening of the ψ -function due to temperature increase.

Source: (Stacey, 2007)

In this study, Doppler broadening as a result of setting temperature conditions at CZP to HFP impacts on the cross-section data of materials present in the MHTGR-350 fuel pin cell, and these will also influence selected output parameters of interest, specifically the k_{inf} . The extent to which it impacts on this cross-section data will be reflected in the results obtained.

3.6 The SCALE 6.1 code system

The SCALE 6.1 (Standardized Computer Analyses for Licensing Evaluation) code was developed at Oak Ridge National Laboratory (ORNL) with the primary goal for modelling and simulation of nuclear reactor systems to enhance their design and safety aspects through reactor physics, criticality and radiation shielding applications (Oak Ridge National Laboratory, 2011). For this study, it is utilized for criticality studies of the MHTGR-350 pin cell. This analysis is performed by a series of executions of computational codes using a few input models. The SCALE 6.1 code system consists of computational codes referred to as modules, and these are further classified as control modules and functional modules. A functional module calculates parameters related to criticality, depletion and or sensitivity and uncertainty analysis. A control module guides a sequence of calculations performed by functional modules and manages the transfer of data between functional modules involved. Functional and control module types within the SCALE 6.1 code package that are utilized in this study are shown in Table 11.

Table 11 - Sample of modular SCALE 6.1 codes used in this study.

Mode	Control module	Executed functional modules					
MG	CSAS6	BONAMI	CENTRM/PMC/WORKER	XSDRNPM	KENO-VI (forward)		
CE	CSAS6				KENO-VI (forward)		
MG	TSUNAMI -3D-K6	BONAMIST	CENTRM/PMC/WORKER	XSDRNPM cellmix	KENO-VI (forward)	KENO-VI (adjoint)	SAMS 6

The functions performed by the above-mentioned functional modules are summarised as follows (SCALE Manual):

- BONAMI = Provides resonance corrected cross-sections in the unresolved resonance range.
or
BONAMIST
- CENTRM = Creates sets of pointwise continuous fluxes based on unit cell description and pointwise continuous energy (CE) cross-section library.
- PMC = Creates a multigroup (MG) cross-section library based on the unit cell description, pointwise continuous cross-section library and a set of pointwise continuous fluxes created by CENTRM.
- WORKER = Reads cross-section libraries formatted as AMPX master or working libraries and produce new AMPX working libraries in a format which is compatible with XSDRNPM, CENTRM, KENO-VI and NEWT.
- XSDRNPM = Calculates the cell-averaged cross-sections when CELLMIX = is specified in the unit cell.
- SAMS 6 = Calculates the sensitivity coefficients of the multiplication factor of a system due to perturbations of the cross-section data together with the uncertainty due to the cross-section covariance data.

The KENO-VI and TSUNAMI-3D modules are described in the following sections, since the primary focus of this study entails extensive use of these codes. The module and code terms are used interchangeably in this work.

3.6.1 The KENO-VI functional module

KENO-VI is a Monte Carlo criticality safety calculation code which was developed at Oak Ridge National Laboratory (Hollenbach, 2011). It is run using the control module CSAS6 (Criticality Safety Analysis Sequence with KENO-VI). It performs the continuous and multigroup criticality calculations using an ENDF-B nuclear data file included in SCALE 6.1 (a version of ENDF-BVII.0 is utilized in this study). When used in multigroup mode, the group cross-sections are prepared by the modules BONAMI, CENTRM, PMC, WORKER and XSDRNPM. These modules are automatically called when using the control module CSAS6.

KENO-VI is capable of modelling three-dimensional systems with complex geometries using sets of quadratic equations using a generalized geometry scheme known as the SCALE 6.1 Generalized Geometry Package (SGGP). Provision for 2D and 3D interactive plots is available for KENO-VI using KENO3D. The outputs after simulations done in KENO-VI can be viewed as text files and also with an HTML-formatted output interface. GeeWiz (Graphically Enhanced Editing Wizard) is a Windows programme that has been developed in SCALE 6.1 and can be used as an alternative to creating and executing input files for KENO-VI. GeeWiz also supports the creation and execution of depletion, burnup, sensitivity and uncertainty calculations that can be run with specific modules of SCALE 6.1.

3.6.2 TSUNAMI-3D control module

TSUNAMI-3D (Tools for Sensitivity and Uncertainty Analysis Methodology Implementation in three dimensions) is a control module of SCALE 6.1 which guides a sequence of calculations performed by respective functional codes as highlighted in Table 11 (Rearden B. T., 2011). These control modules further facilitate the application of sensitivity and uncertainty analysis through execution of the SAMS 6 functional module. The current SCALE 6.1 version of TSUNAMI-3D can only be applied to multigroup calculations.

Sensitivities are ranked by sensitivity coefficients which can be used to predict relative changes in the eigenvalue k due to changes in nuclear reaction probabilities Σ_x i.e. the cross-sections. Mathematically, this is represented as (Perfetti, 2012):

$$S_{k,\Sigma_x} = \frac{\delta k/k}{\delta \Sigma_x/\Sigma_x} \quad (10)$$

Representing the nuclear data parameters by the vector α , the sensitivity coefficients are combined with the cross-section covariance data to find the uncertainties in k due to uncertainties in cross-section data by the equation:

$$\sigma_k^2 = S_k C_{\alpha\alpha} S_k^T \quad (11)$$

This gives the variance in the system's k where S_k is a row vector containing the relevant sensitivity coefficients for the system and $C_{\alpha\alpha}$ is the matrix containing relative variance and covariance of nuclear data. T represents a transpose. $C_{\alpha\alpha}$ is defined as:

$$C_{\alpha\alpha} = \frac{COV(\alpha_x, \alpha_y)}{\alpha_x \alpha_y} \quad (12)$$

where the x and y subscripts vary across the regions, isotopes, energy and reactions of interest and $cov(\alpha_x, \alpha_y)$ is the covariance defined in Equation (3). Generation of sensitivity coefficients and the quantification of uncertainties are described in more detail under Section 3.7. The sensitivity and uncertainty information from SAMS 6 can be viewed in a user-interactive html format which includes results such as sensitivity coefficients by region, nuclide mixture and sensitivity data plots, with uncertainty information due to cross-section covariance given as relative standard deviations (Rearden B. T., 2011).

3.7 Sensitivity analysis

A full body of sensitivity parameters as determined from the neutron-nuclide reactions types (e.g. capture, scatter, total and fission cross-sections) are selected automatically by executing the SAMS 6 functional module. The parameters that greatly influence response parameter values are identified using their sensitivity coefficients. The sensitivity coefficients are calculated by SAMS 6 using a linear perturbation theory approach, which requires the solutions of forward and adjoint flux moments, ϕ and $\phi^\dagger$ respectively (Rearden B. T., 2011).

SAMS 6 calculates the sensitivity coefficients and these are partitioned into explicit sensitivity and implicit sensitivity coefficients. Explicit sensitivity coefficients reflect how a response parameter (e.g. k_{inf}) changes due to related multigroup cross-section change. Implicit sensitivity coefficient reflects how multigroup cross-sections are affected by calculations of the resonance self-shielding effects.

3.7.1 Quantification of uncertainties by use of sensitivity coefficients

Uncertainty input parameters that cause the uncertainty in output parameters of the MHTGR-350 fuel pin cell (Strydom & Bostelmann, Prismatic HTGR Benchmark Definition: Phase 1 INL/LTD-15-34868, June 2015) model arise from:

- Nuclear parameters which are propagated using the multigroup cross-section covariance matrix.
- Manufacturing uncertainties e.g. fuel pin cell dimensions, nuclide densities etc.
- Methods and modelling approximations used in KENO-VI code.
- Selection of the multigroup structure (which approximates the reference continuous energy as discrete groups).
- Double-heterogeneity and self-shielding treatment.

Specifically, the nuclear properties of materials of the fuel pin cell have associated uncertainties which are given in the ENDF-B-VII data library as variance-covariance matrices. These are used as input parameters and can cause values of output parameters of interest mentioned earlier to deviate from their desired values. The single effects due to individual uncertain input parameters are investigated i.e. sensitivity analysis. In addition, the total combined effects of the parameters are calculated i.e. uncertainty analysis. The input parameters that greatly influence the selected outputs are ranked by use of sensitivity coefficients.

3.7.2 Generation of sensitivity coefficients.

In this study, sensitivity coefficients are determined by making use of the adjoint-based perturbation method, and these coefficients reflect the relative change in the system's eigenvalue due to small perturbations in system parameters. This can be derived from the use of steady-state Boltzmann neutron transport equation of the form (Perfetti, 2012):

$$[A - \lambda B]\phi = 0 \quad (13)$$

where ϕ is the neutron flux, $\lambda = 1/k$, A is the neutron transport operator excluding the fission source term, and B is the operator for the fission source term which are given by:

$$A\phi = \vec{\Omega} \cdot \nabla \phi(\vec{X}, E, \vec{\Omega}) + \Sigma_t(\vec{X}, E) \phi(\vec{X}, E, \vec{\Omega}) - \int_{4\pi} d\vec{\Omega}' \int_0^\infty dE' \Sigma_s(\vec{X}, E' \rightarrow E, \vec{\Omega}' \rightarrow \vec{\Omega}) \phi(\vec{X}, E', \vec{\Omega}') \quad (14)$$

$$B\phi = \frac{\chi(\vec{X}, E)}{4\pi} \int_{4\pi} d\vec{\Omega}' \int_0^\infty dE' \bar{v} \Sigma_f(\vec{X}, E', \vec{\Omega}') \phi(\vec{X}, E', \vec{\Omega}') + S(\vec{X}, E, \vec{\Omega}) \quad (15)$$

The respective adjoint and perturbed transport equations can be obtained from Equation (13) as:

$$[A^\dagger - \lambda B^\dagger] \phi^\dagger = 0 \quad (15)$$

$$[A' - \lambda' B'] \phi' = 0 \quad (16)$$

In eigenvalue problems, the neutron source term $S(\vec{X}, E, \vec{\Omega})$ is equal to zero. The perturbed transport operators, eigenvalue and the flux are defined as: $A' = A + \delta A$, $B' = B + \delta B$, $\lambda' = \lambda + \delta \lambda$ and $\phi' = \phi + \delta \phi$. Multiplying Equation (16) by $\phi^\dagger$, integrating over all space $\langle \cdot \rangle$, energy, direction, and expanding the result in terms of the perturbed operators and the eigenvalues gives:

$$\begin{aligned} \langle \phi^\dagger A \phi \rangle + \langle \phi^\dagger \delta A \phi \rangle + \langle \phi^\dagger A \delta \phi \rangle + \langle \phi^\dagger \delta A \delta \phi \rangle \\ = \langle \lambda \phi^\dagger B \phi \rangle + \langle \lambda \phi^\dagger \delta B \phi \rangle + \langle \delta \lambda \phi^\dagger B \phi \rangle + \langle \delta \lambda \phi^\dagger \delta B \phi \rangle + \langle \lambda \phi^\dagger B \delta \phi \rangle \\ + \langle \lambda \phi^\dagger \delta B \delta \phi \rangle + \langle \delta \lambda \phi^\dagger B \delta \phi \rangle + \langle \delta \lambda \phi^\dagger \delta B \delta \phi \rangle \end{aligned} \quad (17)$$

Ignoring higher-order terms above gives:

$$\begin{aligned} \langle \phi^\dagger A \phi \rangle + \langle \phi^\dagger \delta A \phi \rangle + \langle \phi^\dagger A \delta \phi \rangle \\ = \langle \lambda \phi^\dagger B \phi \rangle + \langle \lambda \phi^\dagger \delta B \phi \rangle + \langle \delta \lambda \phi^\dagger B \phi \rangle + \langle \lambda \phi^\dagger B \delta \phi \rangle \end{aligned} \quad (18)$$

By using the property of adjointness $\langle \phi^\dagger (A - \lambda B) \phi \rangle = \langle \phi' (A^\dagger - \lambda^\dagger B^\dagger) \phi^\dagger \rangle$ Equation (18) reduces to:

$$\delta \lambda = \frac{\langle \phi^\dagger (\delta A - \lambda \delta B) \phi \rangle}{\langle \phi^\dagger B \phi \rangle} \quad (19)$$

Given that $\lambda = 1/k \Rightarrow \delta \lambda = -\delta k/k^2$ and, by making use of Equation (10) and Equation (19), the sensitivity of $k = k_{inf}$ due to perturbation of macroscopic cross-section Σ can be expressed as:

$$S_{k, \Sigma_x} = \Sigma_x \frac{\langle \phi^\dagger \left(\lambda \frac{\delta B}{\delta \Sigma_x} - \frac{\delta A}{\delta \Sigma_x} \right) \phi \rangle}{\lambda \langle \phi^\dagger B \phi \rangle} = \frac{T_{1x}(z, E) + T_{2f}(z, E \rightarrow E') + T_{3s}(z, E \rightarrow E')}{D} \quad (20)$$

The physical meaning of the T-terms above and the denominator D is explained in the next section.

These methodologies are implemented in the SAMS 6 functional module of SCALE 6.1 through TSUNAMI-3D model of the MHTGR-350 pin cell. Different types of reactions take place in the pin cell and each one of them impacts on the eigenvalue or multiplication factor of the system. Hence the sensitivity of the multiplication factor to the reactions can be expressed by manipulation of Equation (20) as will be shown in the next Section 3.7.3.

3.7.3 Sensitivity coefficients of the eigenvalue due to reactions

Solutions to Equation (20) require the calculation of the denominator and the numerator, which has three functions (the T-terms) originating from the inner product ϕ and $\phi^\dagger$ with different operators acting on ϕ . The first term, which is the collisional term, describes the forward and adjoint fluxes of the $\Sigma_t(\vec{X}, E)\phi(\vec{X}, E, \vec{\Omega})$ in Equation (14) and is expressed as (Perfetti, 2012):

$$T_{1x}(z, E) = \int_{V_z} \int_{4\pi} \Sigma_x(\vec{X}, E) \phi(\vec{X}, E, \vec{\Omega}) \phi^\dagger(\vec{X}, E, \vec{\Omega}) d\vec{\Omega} dV \quad (21)$$

where z represents a region and V_z is the volume of the region z . The second term is the fission source term in the Equation (20) and is expressed by:

$$T_{2f}(z, E \rightarrow E') = \int_{V_z} \int_{4\pi} \bar{\nu} \Sigma_f(\vec{X}, E) \phi(\vec{X}, E, \vec{\Omega}) d\vec{\Omega} \int_{4\pi} \frac{\chi(\vec{X}, E')}{4\pi} \phi^\dagger(\vec{X}, E', \vec{\Omega}') d\vec{\Omega}' dV \quad (22)$$

where $\vec{\Omega}'$ and E' resembles the neutrons from the fission reactions having random directions and energies. The third term from the inner product of Equation (20) is the scattering source term and is defined as:

$$T_{3s}(z, E \rightarrow E') = \int_{V_z} \int_{4\pi} \int_{4\pi} \phi(\vec{X}, E, \vec{\Omega}) \Sigma_s(\vec{X}, E \rightarrow E', \vec{\Omega} \rightarrow \vec{\Omega}') \phi^\dagger(\vec{X}, E', \vec{\Omega}') d\vec{\Omega}' d\vec{\Omega} dV \quad (23)$$

The denominator term describes the adjoint-weighted fission source term that is integrated for all regions and isotopes and is expressed as:

$$D = \lambda \int_{V_z} \int_0^\infty \int_{4\pi} \bar{\nu} \Sigma_f(\vec{X}, E) \phi(\vec{X}, E, \vec{\Omega}) d\vec{\Omega} dE \int_0^\infty \int_{4\pi} \frac{\chi(\vec{X}, E')}{4\pi} \phi^\dagger(\vec{X}, E', \vec{\Omega}') d\vec{\Omega}' dE' dV \quad (24)$$

The preceding equations have been integrated over the energy and thus the generated sensitivity coefficients are in terms of the multigroup energy.

The following are expressions of sensitivity coefficients according to reaction types (Perfetti, 2012):

1. The capture reaction sensitivity coefficient for the energy group g in a region z :

$$S_{cap}(z, g) = - \int_g \frac{T_{1x=cap}(z, E)}{D} dE \quad (25)$$

2. The fission reaction sensitivity coefficient is expressed as:

$$S_f(z, g) = \int_g \left[\lambda \int_0^\infty \frac{T_{2f}(z, E \rightarrow E')}{D} dE' - \frac{T_{1x=fis}(z, E)}{D} \right] dE \quad (26)$$

3. Scattering reaction sensitivity coefficient is given by:

$$S_s(z, g) = \int_g \left[\int_0^\infty \frac{T_{3s}(z, E \rightarrow E')}{D} dE' - \frac{T_{1x=sca}(z, E)}{D} \right] dE \quad (27)$$

4. The sensitivity coefficient for a nu-bar ($\bar{\nu}$) reaction is given by:

$$S_{\bar{\nu}}(z, g) = \lambda \int_g \left[\int_0^\infty \frac{T_{2f}(z, E \rightarrow E')}{D} dE' \right] dE \quad (28)$$

5. The sensitivity coefficient for the χ reaction is expressed as:

$$S_{\chi}(z, g) = \lambda \int_g \left[\int_0^\infty \frac{T_{2f}(z, E \rightarrow E')}{D} dE' \right] dE \quad (29)$$

These sensitivity coefficients for different reactions are used in this study to rank the different nuclear reactions taking place in the MHTGR-350 fuel pin cell that influence the k_{inf} response parameter change.

3.8 The Reactivity-equivalent Physical Transformation Theory

The reactivity-equivalent physical transformation (RPT) theory is dedicated to converting the double-heterogeneous fuel region (consisting of coated TRISO particles randomly dispersed in graphite matrix) to homogeneous fuel regions. The theory is used because most transport lattice codes do not have the capability for accurate treatment of double-heterogeneous fuel region (Kim, Cho, Lee, Noh, & Zee, 2007). In this study, two approaches by RPT which are the standard and modified methods are applied. In the standard RPT method, the fuel compact radius of the pin cell is kept constant and the matrix graphite is smeared over the whole compact volume. The TRISO particles are smeared and placed in the smaller radius r_{RPT} which must be adjusted to

match the infinite multiplication factor of the reference DOUBLEHET calculation (Rohde, et al., 2012).

In the modified RPT, the TRISO particles are moved into a smaller cylinder of radius r_{RPT} inside the compact and homogenized, while all the matrix graphite fills the remaining space of the fuel compact region (Rohde, et al., 2012). In both these regions the total numbers of isotopes were conserved individually. The number densities of the isotopes in the helium gap and graphite block were conserved individually. This means a mass balance was conserved in all cases.

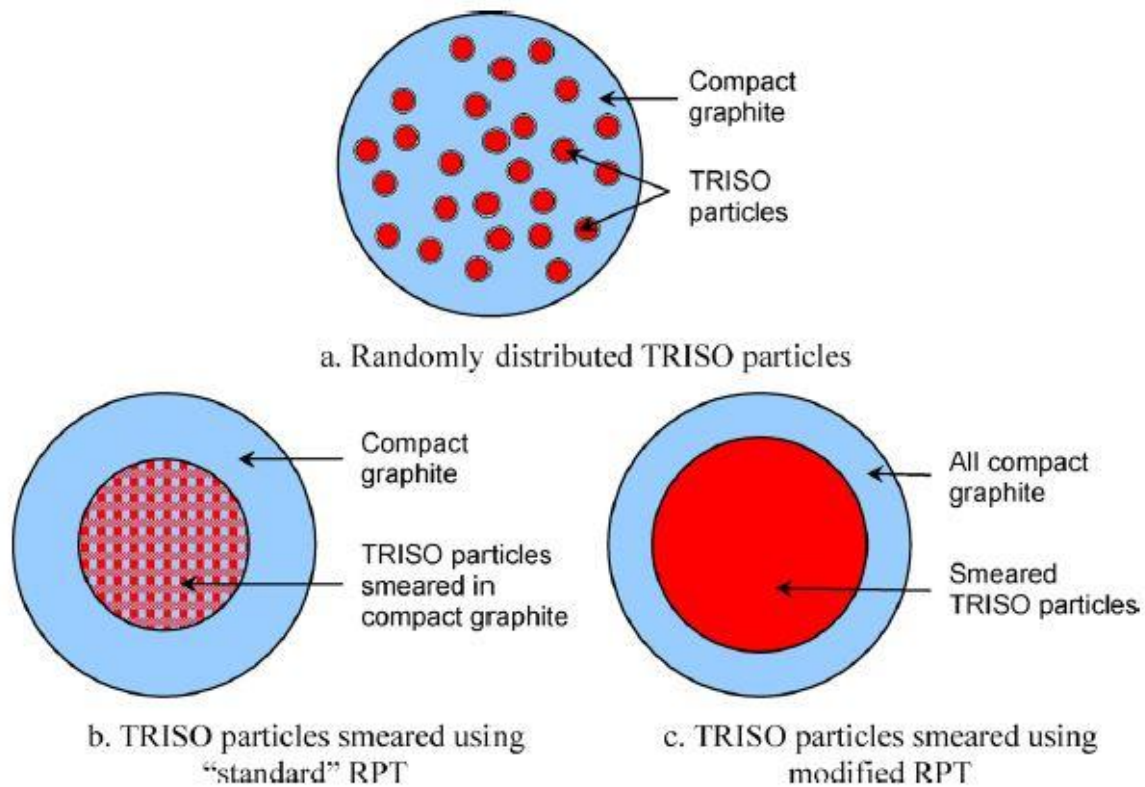


Figure 12 - The standard and modified RPT homogenization techniques.

Source: (Rohde, et al., 2012).

In RPT approaches, the radius r_{RPT} is adjusted by iteration calculations so that the resulting multiplication factor matches that of a reference solution of the double-heterogeneous calculation, which can be obtained from a high-fidelity deterministic code and in Monte Carlo codes. The modified RPT allows for decoupling of TRISO particles and compact graphite matrix temperatures since they occupy different regions. It has been noted that homogenizing the entire fuel compact by volume-weighting underestimates the reactivity due to significant reduction of resonance self-shielding effects of the fuel (Rohde, et al., 2012).

The standard and modified RPT methodologies are applied in KENO-VI and TSUNAMI-3D models of the double-heterogeneous fuel compact of the MHTGR-350 pin cell. Since the

temperatures of all materials in fuel compact are the same as shown in Table 2, the standard RPT is applicable and the results obtained will be compared with those of the modified RPT. The methodology needed to find number densities of isotopes in the RPT models and the adjustment of r_{RPT} to match the reference solution of the double-heterogeneous multiplication factor is discussed later in Chapter 4.

3.9 Convergence criteria of Monte Carlo criticality calculations

The criticality calculations using Monte Carlo techniques (as adopted by KENO-VI in this study) of systems containing fissile material are based on iteration procedures where an initial guess for the fission distribution is specified. There is a need to determine when the solution starts to converge before the eigenvalue and fluxes are collected (Brown, 2006). Inactive and active neutron cycles are therefore specified. Inactive cycles are the neutron generations which are discarded when the distribution has not converged, and active cycles are for generations when uniformity (although statistical in nature) is reached and the tallies are accumulated.

It has been noted that fission distribution converges slower than $k_{inf.}$ convergence (Brown, 2006), hence both these must be simultaneously assessed for convergence to assure correct results. The most effective way to characterize convergence of fission distribution is by use of Shannon entropy.

3.9.1 Eigenvalue convergence

In this section, convergence of the effective multiplication factor $k_{eff.}$ of the system is explained by use of the neutron transport equation. In standard form, the equation is written as follows:

$$\begin{aligned} & [\vec{\Omega} \cdot \nabla + \Sigma_t(\vec{X}, E)]\phi(\vec{X}, E, \vec{\Omega}) \\ &= \iint \phi(\vec{X}, E', \vec{\Omega}') \Sigma_s(\vec{X}, E' \rightarrow E, \vec{\Omega} \cdot \vec{\Omega}') d\vec{\Omega}' dE' \\ &+ \frac{1}{k_{eff.}} \frac{\chi(E)}{4\pi} \iint v \Sigma_f(\vec{X}, E') \phi(\vec{X}, E', \vec{\Omega}') d\vec{\Omega}' dE' \end{aligned} \quad (30)$$

Equation (30) above can be simplified further using operator form according to the following:

$$(L + T)\phi = S\phi + \frac{1}{k_{eff.}} M\phi \quad (31)$$

Rearrangement leads to:

$$\phi = \frac{1}{k_{eff.}} (L + T - S)^{-1} M\phi = \frac{1}{k_{eff.}} F\phi \quad (32)$$

The standard power iteration method can be used to solve Equation (32) as follows (Brown, 2006):

$$\phi^{(n+1)} = \frac{1}{k_{eff}^{(n)}} F \phi^{(n)}, n = 0, 1, \dots, \text{given } k_{eff}^0 \text{ and } \phi^{(0)} \quad (33)$$

During the convergence of k_{eff} and the fission source distribution by power iteration method, $\phi^{(0)}$ can be expressed by utilizing the eigenvectors u_j of Equation (30) i.e. $\phi = \sum_{j=0} a_j^0 \bar{u}_j$. Substituting this in Equation (33) and manipulating the algebra leads to:

$$\phi^{(n+1)}(\bar{r}) = \bar{u}_0(\bar{r}) + \frac{a_1}{a_0} \rho^{n+1} \cdot \bar{u}_1(\bar{r}) + \dots \quad (34)$$

$$k_{eff}^{(n+1)} = k_0 \cdot \left[1 - \frac{a_1}{a_0} \rho^n (1 - \rho) g_1 + \dots \right] \quad (35)$$

The parameter ρ is called the dominance ratio, defined as (k_1/k_2) , k_0 and $\bar{u}_0$ are fundamental eigenvalue and eigenfunction respectively. The first mode eigenvalue and eigenfunctions are denoted as k_1 and $\bar{u}_1$ accordingly, and a_0 , a_1 and g_1 are the constants which are determined by expansion of initial fission source distribution. When a value for ρ is close to 1, k_{eff} converges faster than fission source distribution because of a damping factor $(1 - \rho)$ that is close to zero. This emphasizes the point that convergence of both fission source distribution and the k_{eff} should be monitored before Monte Carlo results are accumulated (Brown, 2006).

3.9.2 Fission source convergence by Shannon entropy

Convergence of the fission source distribution is assessed by use of the Shannon entropy H_{src} in selected MCNP Monte Carlo codes (Brown, 2006). As the source distribution converges, the H_{src} values tend to assume common results or approach uniformity. Calculation of H_{src} involves dividing the 3D system into grid geometry and tallying the number of fission sites in a cycle (i.e. neutron generation) belonging to a particular grid. Given that:

$$N_s = \text{Number of grid boxes in a mesh.}$$

$$P_j = \frac{\text{Number of source sites in } j^{\text{th}} \text{ mesh element}}{\text{Total number of source sites}}$$

The Shannon entropy H_{src} can be calculated by the equation:

$$H_{src} = - \sum_{j=1}^N P_j \ln_2(P_j) \quad (36)$$

Plots of H_{src} versus neutron generations are provided by some MCNP codes after a simulation is complete (Brown, 2006), together with the average and population standard deviation of H_{src} . When a plot is provided, it is easier to deduce an initial number of neutron generations that should be skipped to facilitate a convergence study, including the convergence of system's k_{inf} .

Source distribution convergence of the MHTGR-350 fuel pin cell is studied in parallel using the MCNP6 code to this study. This was done by the study supervisor since the author is not licensed to use MCNP6. MCNP6 convergence studies were required because KENO-VI is not able to supply source points in the calculation mesh required for computing the Shannon entropy without considerable effort in both model setup and computational time. MCNP6 calculates Shannon entropy for each cycle and further recommends a number of initial neutron generations to be skipped.

CHAPTER 4 – METHODOLOGY AND STUDY APPROACH

4.1 Introduction

In this Chapter, the steps followed to install and run calculations in SCALE 6.1 are described. Procedures to build the IAEA CRP MHTGR-350 fuel pin cell models in the KENO-VI and TSUNAMI-3D codes are presented. The unique input file specifications in these codes with regard to homogeneous, double-heterogeneous and RPT approach are further presented.

4.2 Installing and running the SCALE 6.1 code

Verification was done that the computing system used in this study satisfies the system requirements for installation of SCALE 6.1. Properties of the computing system used in this study are as follows: Windows 7, 64-bit Operating System, 4 GB RAM, Intel(R) Core(TM) i3-3110M CPU @ 2.40 GHz processor. The following steps were then followed as part of guidelines for installation:

- a) Java Runtime Environment (64-bit file) was downloaded and installed: jre-7u75-windows-x64.
- b) Four SCALE 6.1 discs were installed in the C:\scale6.1 path directory, consecutively after every prompt request to insert and install the discs.
- c) When installation was complete, the time and date settings of computing system were modified from the following directories:

Windows start > Control panel > Clock, Language and Region > Date and Time > Change Date and Time Settings > Change calendar settings > Customize Format > Time and Date.

Time and Date tabs appeared:

Time	short time	h/H
	long time	h/H
Date	short date	dd/MM/yyyy
	long date	dd MMMM yyyy

The short time and short date were changed to 2/14 and 25/08/2014, respectively.

- d) The SCALE 6.1 package comes with the input files of example sample problems and their respective results in output files. A test was thus made to verify that SCALE 6.1 was installed properly by running the input file of a sampled problem and comparing it with the provided results in the output file.

For example, a sample problem with a filename csas6_1.input stored in C:\scale6.1\smplprbs\Windows directory was run using the following commands in the Command Prompt:

```
C:\scale6.1\smplprbs\Windows\batch6.1.bat csas6_1
```

The output when the simulation was completed was stored in the same directory as the input file, and this was compared with the supplied output results csas6_1.output stored in the C:\scale6.1\output directory.

After comparison, confirmation was done that SCALE 6.1 had installed successfully and the results were correctly reproduced.

4.3 KENO-VI models of the MHTGR-350 fuel pin cell

The benchmark specification of the IAEA CRP MHTGR-350 fuel pin cell has been provided as can be seen in Section 2.3. To carry on with the analysis so as to give a feedback on the problem statement, the computational resources are utilized which provide a platform to model the MHTGR-350 fuel pin cell. For this, KENO-VI functional module of SCALE 6.1 is used. At this stage, KENO-VI is used to provide base value or nominal calculations and the next level for the sensitivity and uncertainty analysis will be performed by the TSUNAMI-3D model of the MHTGR-350.

4.3.1 Homogeneous model

The homogeneous KENO-VI model of the MHTGR-350 fuel pin cell input file is included in Appendix A. Section A1. This file was built as follows:

- a) **Control module:** CSAS6

The control module guides the sequence of the calculations to be performed for solving the problem. In this case, CSAS6 was selected and the sequences of calculations are shown in Table 11.

- b) **Problem title:** The homogeneous KENO-VI model of the MHTGR-350 fuel pin cell

This identifies the type of problem at hand for which the solution is required.

c) **Cross-section library:** v7-238

This indicates that the seventh version of the ENDF nuclear data library (ENDF-B-VII.0) was used, and the 238 multigroup energy scheme was used for the calculation.

d) **Material composition**

In this block, the isotopes, number densities and temperatures (CZP state) of the materials of MHTGR-350 fuel pin cell were specified. The compositions belonging to the fuel compact, helium coolant channel and H-451 block graphite were assigned mixture numbers 1, 2 and 3 respectively for identification. The number density of every isotope was defined following Table 5.

e) **Celldata:** Triangular pitch

In this block, the unit cell type is specified as a TRIANGPITCH. The geometry of this unit cell together with the order of arrangement of materials within is shown in Figure 13:

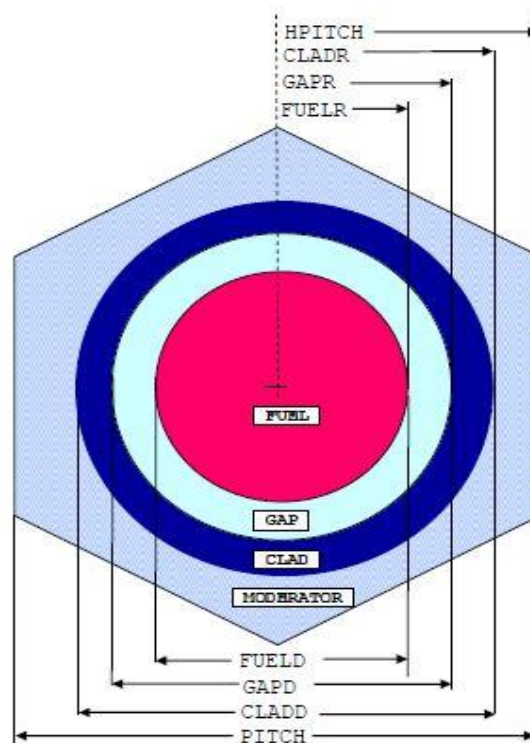


Figure 13 - TRIANGPITCH unit cell and the arrangement of materials.

Source: (SCALE 6.1 Manual).

Using this unit cell type for the homogeneous KENO-VI model of MHTGR-350 pin cell, the arrangement of materials and dimensions of the triangular pitch cell is specified as:

Fuel compact outer radius = FUELR = 0.6225 cm

Helium gap outer radius = GAPR = 0.6350 cm.

Unit cell pitch = HPITCH = 0.9398 cm.

The composition belonging to FUELR was identified as 1, composition in GAPR was 2, and the composition in HPITCH was 3. This was consistent with the labelling as described in d) above.

Also specified is the CENTRM data containing ISN and SZF used for cross-section processing. These are discussed in detail in Chapter 5.

f) **Parameter block**

This block allows the control of the calculations for how it should run, when it should terminate and also serves as a platform for requesting a number of outputs to be generated after the simulation completes. Requested outputs for this MHTGR-350 homogeneous model include the flux, fission number densities, mesh fluxes, and system k_{inf} . amongst a few. Values for NPG, NSK, GEN and SIG are specified in such a way that the Shannon entropy of the source distribution and the k_{inf} . converge. The NPG, NSK, GEN and SIG parameters are discussed in detail under Chapter 5.

g) **Mixing table:** SCT = -1

The cross-section mixing table for the defined mixtures used in this MHTGR-350 fuel pin cell is entered here and is characterized by the SCT parameter. The SCT is the number of discrete scattering angles and was ascribed a value of -1. This implies that the number of scattering angles is determined using the highest order possible as specified on the library.

h) **Geometry block**

In this block, the different units with defined geometric shapes such as hexagons, cylinders, spheres, planes etc. are input so as to build the MHTGR-350 pin cell as a global unit. The isotopes that are contained in each of the units are specified using the mixture numbers as described in d) above. This geometry block is shown in Appendix A. Section A1. KENO-VI input file, between lines 43 and 53. The way in which each unit was defined is as follows:

The 3D co-ordinate axes were located at the centre of all units by default. Cylinder 1, representing the fuel compact, was assigned a radius of 0.6225 cm, the height in the positive z-axis of 2.464 cm and height in the negative z-axis of -2.464 cm i.e. since the total height of the unit cell is $z = 4.928$ cm. Cylinder 2, representing the gap between the compact and the matrix graphite block was assigned a radius of 0.635 cm. Rhexprism 3 represents the hexagonal block graphite,

which is rotated as in Figure 5a and encloses Cylinder 2. The pitch of the rhexprism 3 is $p_{pitch} = 0.9398$ cm.

The composition labelled 1 is placed inside cylinder 1 (media 1 1 1), composition 2 is placed inside cylinder 2 outside cylinder 1 (media 2 1 2 -1), and composition 3 is contained inside rhexprism 3 outside cylinder 2 (media 3 1 3 -2). The volume calculation for each region can be performed analytically or by use of GeeWiz and KENO3D by clicking the KENO3D Volumes button. The volumes for each region are required for calculations of the fission densities, fluxes etc. The outer boundary for the fuel pin cell model is rhexprism 3.

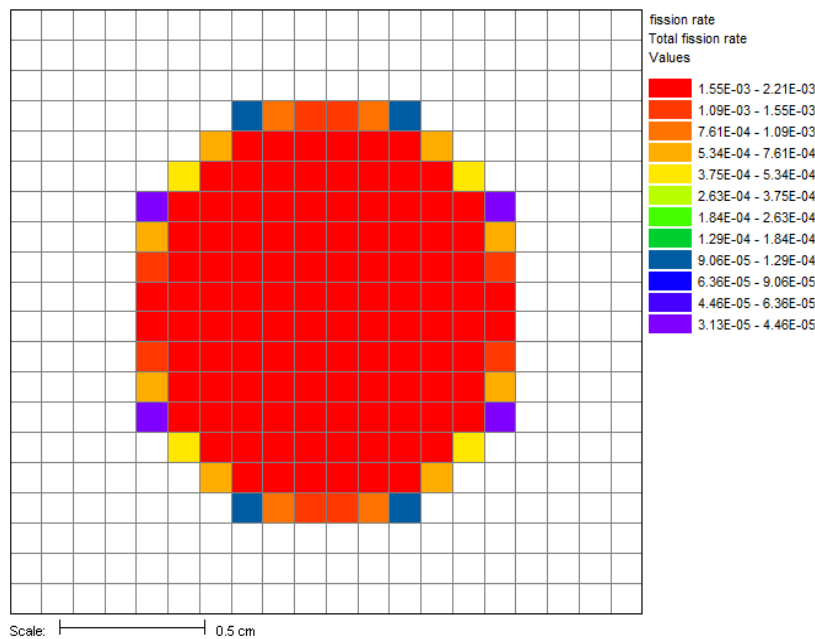
i) **Boundary condition:** Reflected

It was assumed that the MHTGR-350 fuel pin cell is surrounded by identical pin cells of the same type in all six symmetry directions of the hexagon. Thus, as will be seen in the results section, the criticality is calculated as infinite multiplication factor k_{inf} .

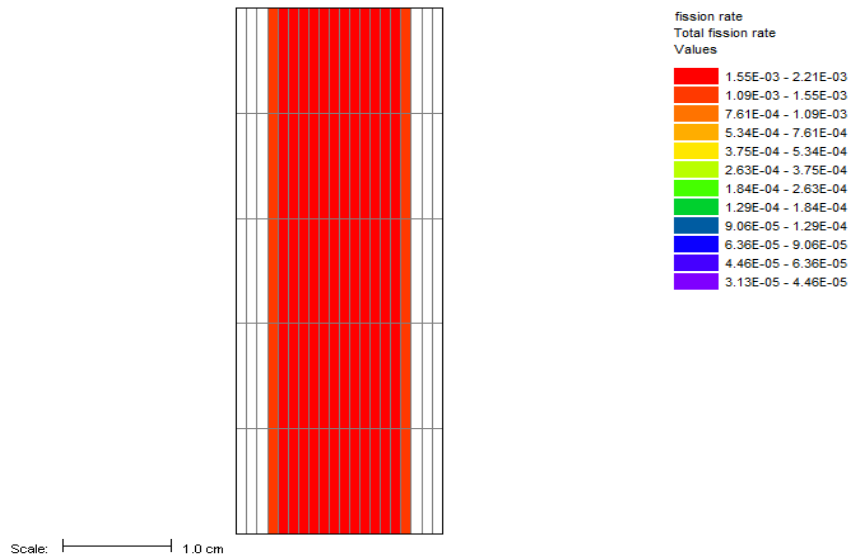
j) **Gridgeometry block**

The MHTGR-350 pin cell model was divided into 20 mesh intervals along its x and y co-ordinate axes, and into 5 mesh intervals along the z axis. A cuboid enclosing this global MHTGR-350 pin cell model was assigned the following dimensions: -X = -1.08519 cm, +X = 1.08519 cm, -Y = -0.9398 cm, +Y = 0.9398 cm, -Z = -2.464 cm, and +Z = 2.464 cm. This mesh allows for calculating fluxes within each grid box and thus to calculate fission rates in the grid boxes, as can be seen in Figure 14 below.

a). Top view (x-y plane).



b). Side view (y-z plane).



c). Front view (x-z plane).

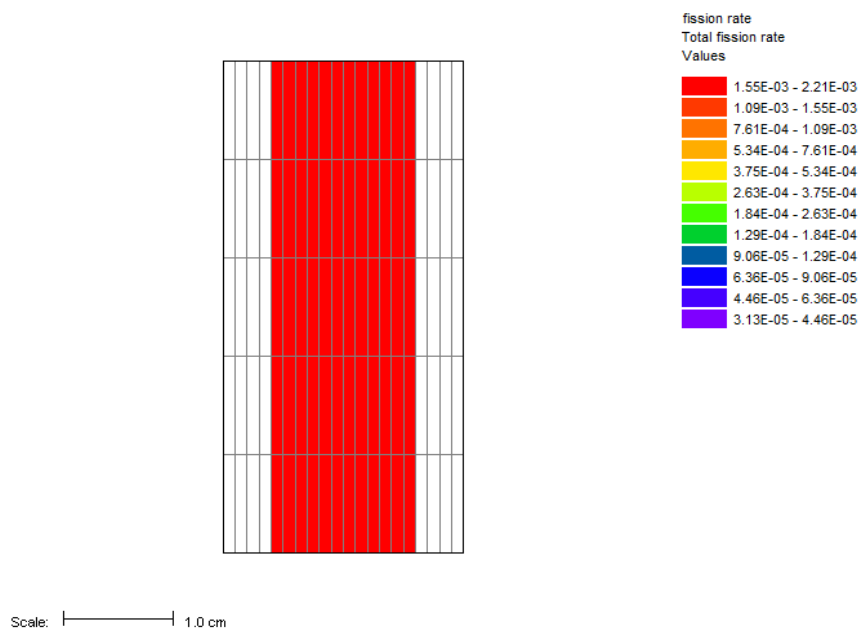


Figure 14 - Mesh views of the MHTGR-350 fuel pin cell model.
Source: (Obtained using the Mesh File Viewer of the SCALE 6.1).

This concludes the procedure for the development of the KENO-VI homogeneous model of MHTGR-350 fuel pin cell using 238 multigroup cross-section library at CZP state. The other model at HFP state was built by only changing temperatures in the Material composition block.

A similar structure again for the continuous energy cross-section library was set up by replacing v7-238 with ce_v7_endf. In this case, the Celldata block was not used. The CZP and HFP states of the continuous energy cross-section library were built. Figure 15 below shows the KENO-VI homogeneous model of the MHTGR-350 fuel pin cell.

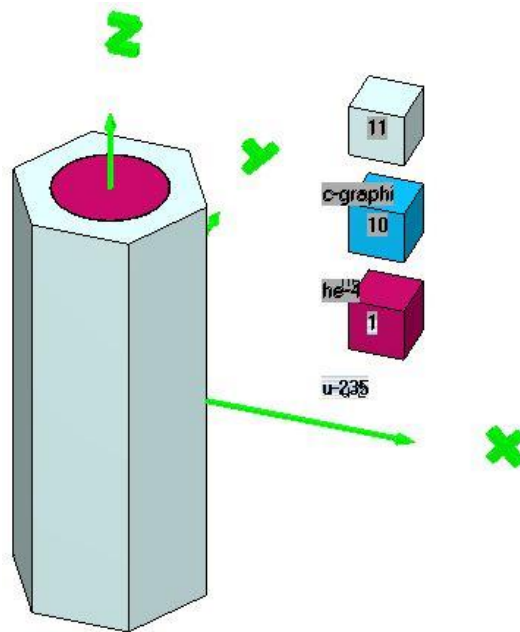


Figure 15 - KENO-VI homogeneous model of the MHTGR-350 fuel pin cell.

Source: (Obtained from KENO3D).

4.3.2 Double-heterogeneous model

To construct this model, the following changes or additional data were made following the one described in Section 4.3.1:

Problem title: The double-heterogeneous KENO-VI model of the MHTGR-350 fuel pin cell

Cross-section library: v7-238

The current version of SCALE 6.1 used in this study only allows calculations of the double-heterogeneous KENO-VI model using the multigroup energy. The v7-238 cross-section library of the ENDF-B-VII.0 was used.

Material composition

The isotopes and number densities were changed to those outlined in Table 6.

Compositions belonging to UCO Kernel of TRISO particle were assigned the mixture number of 1, composition in Porous carbon buffer layer as mixture 2, composition in Inner PyC as mixture 3, composition in SiC as mixture 4 and composition in Outer PyC as mixture 5.

The composition of graphite matrix in which the TRISO particles are dispersed was assigned the mixture number 6, composition of helium coolant channel as mixture 7 and H-451 block graphite as mixture 8.

Temperature conditions at CZP and HFP are set within this block.

Cell data

Within this block the DOUBLEHET cell for the unit cell was provided, in addition to TRIANGPITCH unit cell type. The DOUBLEHET cell allows for specifying the TRISO particle structure, dimensions of the coating layers, isotopes within each layer, the volume fraction of TRISO particles in the fuel compact, and also labelling the matrix in which the particles are dispersed, as shown in Figure 16 below.

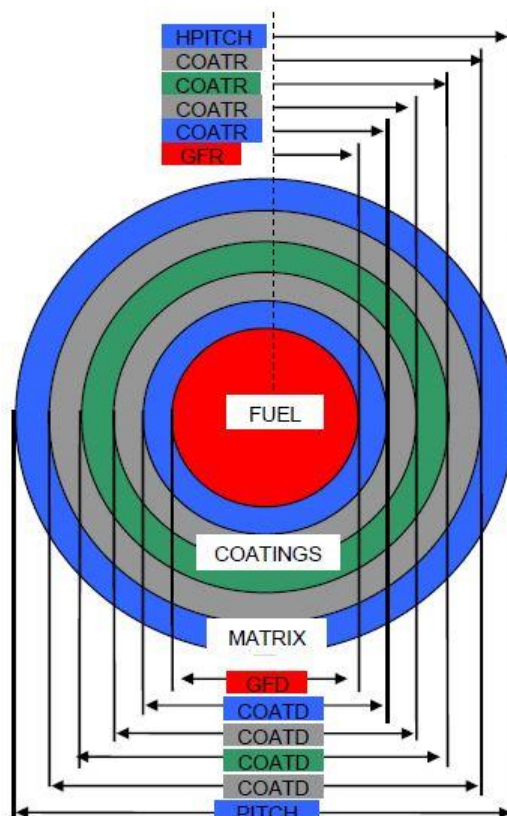


Figure 16 - TRISO particle model structure and the arrangement of materials.

Source: (SCALE6.1 Manual).

The specifications for DOUBLEHET in conjunction to KENO-VI double-heterogeneous model were specified in reference to Table 4 as follows:

UCO Kernel radius = GFR = 0.02125 cm

Porous carbon buffer layer outer radius = COATR = 0.03125 cm

Inner PyC outer radius = COATR = 0.03525 cm

SiC outer radius = COATR = 0.03875 cm

Outer PyC outer radius = COATR = 0.04275

The compositions for the fuel kernel and all other layers were defined using unique mixture numbers. The labelling of composition numbers were in line with those described in the Material composition block above. The average TRISO particle volume fraction was set as: $vf = 0.35$.

The remaining blocks not described here retain the same settings as those highlighted in Section 4.3.1.

Two models at CZP and HFP states of the double-heterogeneous KENO-VI model of the MHTGR-350 were obtained, all using the v7-238 cross-section library.

4.4 RPT homogenization of the MHTGR-350 in KENO-VI

This section presents the homogenization techniques of the RPT, which are the standard and modified RPT methods of the double-heterogeneous MHTGR-350 fuel pin cell. In the standard RPT method, the matrix graphite is smeared throughout the compact and a portion of this is smeared together with the TRISO particles in a smaller cylinder of adjustable radius r_{RPT} , while in the modified RPT method all the matrix graphite fills the space outside the smaller cylinder radius r_{RPT} (containing only smeared TRISO particles) inside the compact. These are only built using the v7-238 cross-section library to allow for further extension into the TSUNAMI-3D code.

4.4.1 The standard RPT model

This model is similar in structure to that described in Section 4.3.1. Modifications are as follows:

Problem title: The standard RPT KENO-VI model

Material composition

The procedures of the standard RPT theory followed in converting the double-heterogeneous model number densities described in Section 4.3.2 to homogenized number densities are as follows:

- a) The number densities of all isotopes present in the fuel region shown in Table 6, given as [atoms/b·cm] were converted to units of [atoms/cm³] through multiplication by 10²⁴ i.e. 1 barn = 10⁻²⁴ cm².
- b) The volumes of the coating-layers of the Kernel, Porous carbon buffer, iPyC, SiC and oPyC were calculated as follows:

$$\begin{aligned}V_{\text{Kernel}} &= \frac{4}{3} \cdot \pi \cdot r_{\text{Kernel}}^3 \\V_{\text{Buffer}} &= \frac{4}{3} \cdot \pi \cdot r_{\text{Buffer}}^3 - V_{\text{Kernel}} \\V_{\text{iPyC}} &= \frac{4}{3} \cdot \pi \cdot r_{\text{iPyC}}^3 - [V_{\text{Buffer}} + V_{\text{Kernel}}] \\V_{\text{SiC}} &= \frac{4}{3} \cdot \pi \cdot r_{\text{SiC}}^3 - [V_{\text{iPyC}} + V_{\text{Buffer}} + V_{\text{Kernel}}] \\V_{\text{oPyC}} &= \frac{4}{3} \cdot \pi \cdot r_{\text{oPyC}}^3 - [V_{\text{SiC}} + V_{\text{iPyC}} + V_{\text{Buffer}} + V_{\text{Kernel}}]\end{aligned}$$

The radii of each of the coating layers are summarised in Table 4.

- c) The volumes of each region of the fuel compact, helium coolant channel and graphite block were calculated as follows:

$$\begin{aligned}V_{\text{comp.}} &= \pi \cdot r_{\text{comp.}}^2 \cdot h_{\text{comp.}} \\V_{\text{channel}} &= \pi \cdot r_{\text{channel}}^2 \cdot h_{\text{comp.}} - V_{\text{comp.}} \\V_{\text{block}} &= \frac{\sqrt{3}}{2} \cdot p_{\text{pitch}}^2 \cdot h_{\text{comp.}} - [V_{\text{comp.}} + V_{\text{channel}}]\end{aligned}$$

In the above, $h_{\text{comp.}}$ and p_{pitch} are the fuel compact height and the unit cell pitch, respectively, as also seen in Table 4.

- d) Total volumes occupied by TRISO particles and graphite matrix in the fuel compact were then calculated with use of the average TRISO packing fraction p_{fraction} :

$$V_{\text{TRISO}} = p_{\text{fraction}} \cdot V_{\text{comp.}}$$

$$V_{\text{matrix}} = [1 - p_{\text{fraction}}] \cdot V_{\text{comp.}}$$

The number of TRISO particles in compact was calculated as: $N_{\text{TRISO}} = V_{\text{TRISO}} / \left[\frac{4}{3} \cdot \pi \cdot r_{\text{oPyC}}^3 \right]$ i.e. dividing the total occupied volume of TRISO particles in the compact by the volume of a TRISO particle.

- e) Total volume of the Kernel, Porous carbon buffer, iPyC, SiC and oPyC in the fuel compact were calculated prior to finding numbers of isotopes in the fuel compact as follows:

$$V_{\text{KernelTotal}} = N_{\text{TRISO}} \cdot V_{\text{Kernel}}$$

$$V_{\text{BufferTotal}} = N_{\text{TRISO}} \cdot V_{\text{Buffer}}$$

$$V_{\text{iPyCTotal}} = N_{\text{TRISO}} \cdot V_{\text{iPyC}}$$

$$V_{\text{SiCTotal}} = N_{\text{TRISO}} \cdot V_{\text{SiC}}$$

$$V_{\text{oPyCTotal}} = N_{\text{TRISO}} \cdot V_{\text{oPyC}}$$

- f) The total number of each of the isotopes of materials shown in Table 6 was calculated by multiplying the number density of individual isotopes by their total volumes. Table 12 below shows the ascribed total volumes for each material composition in the MHTGR-350 fuel pin cell.

Table 12 - Total volumes of material compositions in the MHTGR-350 fuel pin cell.

Isotopes belonging to:	Volume used
Kernel	$V_{\text{KernelTotal}}$
Porous carbon buffer	$V_{\text{BufferTotal}}$
iPyC	$V_{\text{iPyCTotal}}$
SiC	V_{SiCTotal}
oPyC	$V_{\text{oPyCTotal}}$
Compact matrix	V_{matrix}
Coolant channel	V_{channel}
H-451 block graphite	V_{block}

- g) The standard RPT model contains four regions and this follows from the description given in Section 3.8. This model is shown in Figure 17. The region 1, defined inside cylinder 1, contains the TRISO particles smeared together with a portion of the matrix graphite and its radius is defined by the r_{RPT} value. Region 2 is inside cylinder 2 outside cylinder 1, and it contains the remaining matrix graphite. The radius of this cylinder 2 is the radius of the original fuel compact and is kept fixed. The last two regions are for the He-4 and c-graphite block and are defined by cylinder 3 and rhexpism 4, respectively. The number densities in these two volumes remain the same since their dimensions are not changed from the benchmark definition. The volumes were defined in the following manner:

Volume for region 1:

$$V_{\text{RPT}} = \pi \cdot r_{\text{RPT}}^2 \cdot h_{\text{comp.}} \quad (37)$$

The r_{RPT} is restricted inside the cylinder 2 i.e. $r_{\text{RPT}} \leq 0.6225$ cm.

Volume for region 2:

$$V_{\text{MatrixRPT}} = \pi \cdot h_{\text{comp.}} \cdot [(0.6225)^2 - (r_{\text{RPT}})^2] \quad (38)$$

The partitioning of the matrix graphite in regions 1 and 2 was made by use of volume fractions. The fraction of matrix graphite contained in region 1 was calculated as $V_{\text{RPT}}/V_{\text{comp.}}$ and the remaining fraction of matrix graphite contained in region 2 was calculated as $V_{\text{MatrixRPT}}/V_{\text{comp.}}$. It should be noted that in region 1 the number densities of graphite material belonging to TRISO particles in the five layers and the portion of matrix graphite are added together.

The volumes of the helium coolant channel and graphite block are the same as those calculated in item c) previously.

- h) The total number of graphite isotopes in region 1 were found by adding the isotopes belonging to the five layers in TRISO particles with a portion of isotopes belonging to compact matrix found in item f), and the region 2 contained the remaining portion of isotopes belonging to compact matrix.

The number density in [atoms/cm³] of all the isotopes in the fuel pin cell are re-calculated by dividing the number of isotopes by the volumes defined for each region. All materials in region 1 are divided by V_{RPT} , matrix graphite isotopes in region 2 are divided by $V_{\text{MatrixRPT}}$, ⁴He number of isotopes are divided by V_{channel} and the c-graphite isotopes in the H-451 block graphite are divided by V_{block} .

These number densities are then converted to [atoms/b·cm] units by dividing with 10^{24} throughout and then input to the Material composition block.

Celldata block: The FUELR, GAPR, CLADR and HPITCH values were specified which contain a TRISO particle mixture and a portion of matrix graphite, the remaining matrix graphite material, the He-4 coolant and the c-graphite of H-451 graphite block respectively. Note that the GAPR was not the gap but the remaining compact matrix c-graphite and that CLADR was the helium gap.

Geometry block: The new dimensions of the units cylinder 1, cylinder 2, cylinder 3 and rhexprism 4 and the volumes in each region were defined. The compositions in the regions defined by these units were determined in the same manner described previously.

The remaining blocks not described here retains the same settings as those highlighted in Section 4.3.1.

When the first two r_{RPT} guess values, say r_1 and r_2 and their respective multiplication factors k_1 and k_2 have been found but none matches the reference $k_{\text{inf.}}(\text{Ref.})$ closely, a new r_{RPT} value called r_i can be found by interpolation methods using the following equation:

$$\frac{k_2 - k_1}{r_2 - r_1} = \frac{k_i - k_1}{r_i - r_1} \quad (39)$$

This value can then be used to calculate the model with new specification, and the k_i obtained. The requirement used in this study is that: $|k_{\text{inf.}}(\text{RPT}) - k_{\text{inf.}}(\text{Ref.})| \leq 20 \text{ pcm}$. The procedure is therefore iterated until a k_i is obtained within the required precision.

Thus two standard RPT KENO-VI models of MHTGR-350 pin cell built in this manner are obtained, one at CZP and the other at HFP all using the 238 cross-section library.

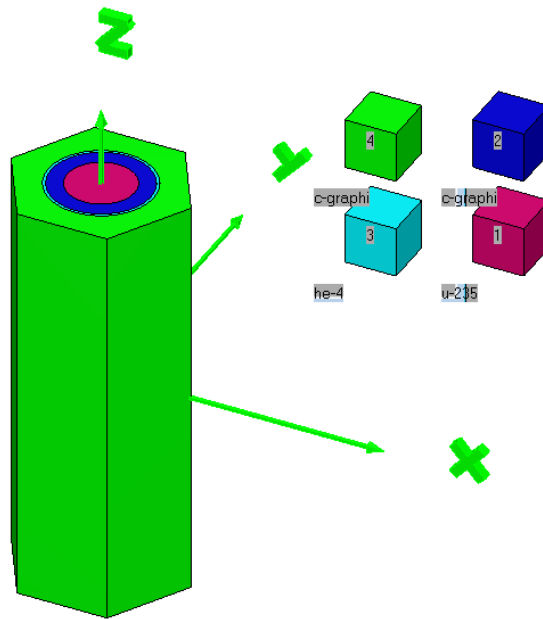


Figure 17 - The standard RPT KENO-VI model of the MHTGR-350 pin cell.

Source: (Obtained from KENO3D).

4.4.2 The modified RPT model

This model is similar in structure to that described in Section 4.3.1. Modifications are as follows:

Problem title: The modified RPT KENO-VI model

Material composition

The procedure to obtain the number of isotopes and the density in the modified RPT method is the same as the one described in Section 4.4.1 except that the whole of the matrix graphite isotopes are contained in region 2 i.e. volume fraction of the matrix graphite in region 1 is zero and it is one in region 2. The geometrical configuration for this model is similar to the one shown in Figure 17.

The remaining blocks not described here retain the same settings as those highlighted in Section 4.3.1.

Thus two modified RPT KENO-VI models of MHTGR-350 pin cell are obtained, one at CZP and the other at HFP all using the 238 cross-section library.

4.5 TSUNAMI-3D models of the MHTGR-350 fuel pin cell

This section provides additional information that is required with the use of the TSUNAMI-3D to that required using KENO-VI models. This is the sensitivity and uncertainty data.

4.5.1 The homogeneous TSUNAMI-3D model

To construct this model, the following changes or additional data gathering was done from the one described in Section 4.3.1.

Control module: TSUNAMI-3D-K6

The TSUNAMI-3D-K6 control module guides the sequence of the calculations to be performed for solving the problem, which are shown in Table 11.

Problem title: The homogeneous TSUNAMI-3D model of the MHTGR-350 fuel pin cell

Cross-section library: v7-238

All calculations were done using the multigroup energy and in this case, the v7-238 cross-section library was used.

Parameter block

Sensitivity and uncertainty quantification in TSUNAMI-3D solves the forward and adjoint problems of the system and it is required, under the TSUNAMI-3D guidelines, that final adjoint and forward solutions of the k_{inf} be well converged i.e. agree to within 1000 pcm. To achieve convergence, a large number of generations AGN, generations skipped ASK and neutrons per generations APG for adjoint case were specified in this block. Their values were defined automatically with reference to those used in the forward calculation as: $AGN = GEN - NSK + ASK$, $ASK = 3 \cdot NSK$ and $APG = 3 \cdot NPG$. This is because adjoint solutions require more sampling and also because they converge more slowly in comparison to forward calculations as stipulated under the TSUNAMI-3D guidelines.

SAMS block

In this block control options such as makeimp, pltp, prtgeom, usemom and prtimp are enabled for computation of sensitivity and uncertainty data from using data generated in the resonance self-shielding calculations and in the forward and adjoint criticality calculations. The makeimp option makes implicit sensitivity coefficients, prtgeom and prtimp prints the sensitivity data by geometry region and implicit sensitivity coefficients, respectively. pltp causes the Javapeño-3D file (an interactive plotting program included in SCALE 6.1 code package in 2D and 3D capabilities) that has $\phi\phi^\dagger$ matrices written in the .htmd directory of the output. The usemom control

option causes flux moments that are calculated by KENO-VI to be used in the generation of sensitivity coefficients.

Appendix A. Section A1. shows the above described input file of TSUNAMI-3D homogeneous model.

Thus two TSUNAMI-3D homogeneous models of the MHTGR-350 pin cell are obtained at CZP and HFP states, all using the 238 cross-section library.

4.5.2 The standard and modified RPT TSUNAMI-3D models

The TSUNAMI-3D models of the standard and modified RPT methodology of the MHTGR-350 pin cell follow the same structure as the one described for the homogeneous model with modifications in the problem title. It should be noted that in all TSUNAMI-3D models the overall layout is preserved from the KENO-VI input specification for the respective models and that the control sequence, adjoint and SAMS block parameters are additional.

CHAPTER 5 – RESULTS AND DISCUSSIONS

5.1 Introduction

In this chapter, the results obtained with KENO-VI and TSUNAMI-3D models of the MHTGR-350 fuel pin cell are presented. These are the homogeneous, double-heterogeneous and RPT models all of which are assessed at CZP and HFP states. Comparisons of the models and the discussions thereof are also presented.

Section 5.5 concludes this chapter by verification of the results generated with KENO-VI and TSUNAMI-3D modules.

5.2 KENO-VI simulation convergence

In the following, convergence results of the Shannon entropy of the fission source and the multiplication factor of a system are presented. The convergence of KENO-VI calculations is dependent on the neutrons per generation (NPG), the number of generations (GEN) and initial generations skipped (NSK) and these are investigated in the continuous energy and 238 multigroup energy KENO-VI models of the MHTGR-350 fuel pin cell.

5.2.1 Continuous energy (CE)

The convergence of the Shannon entropy for the fission source distribution was conducted as an independent study outside this work and the results will be presented at PHYSOR-2016 (Naicker, Maretele, Reitsma, Bostelmann, & Strydom, to be published in 2016), as was addressed in Section 3.9.2. It was found that NPG greater than 10000 requires twelve generations to be skipped. It was decided to set NSK to 60 since this value was larger than twelve and did not impact on computational time significantly.

A decision was again made to set NPG equal to 50000 in line with those used by (Strydom & Bostelmann, Prismatic HTGR Benchmark Definition: Phase 1 INL/LTD-15-34868, June 2015). This number is larger than NPG equal to 10000 required when twelve or more generations are to be skipped as stated in the preceding paragraph.

The last parameter, GEN, was chosen such that the standard deviation in k_{inf} was less or equal to 14 pcm. After the analysis of results, the value for GEN satisfying this requirement was pitched at 600.

Three parameters which are the ISN (order of angular quadrature), SZF (spatial mesh factor) and SCT (number of scattering angles) were investigated for total convergence. These parameters were chosen since they are the control parameters that greatly influence the accuracy and

convergence of the KENO-VI and TSUNAMI-3D models. However, since this section describes continuous energy calculations, the ISN and SZF are required by their resonance processing modules in multigroup calculations and thus are not applicable here. An SCT value of -1 was chosen and this implies that the number of scattering angles is determined from the cross-section library specified (ENDF-B-VII.0) using the highest order possible as specified on the library.

These settings were preserved in the KENO-VI model for CE calculations at CZP and HFP temperature conditions.

5.2.2 Multigroup energy (MG)

In this section, the parameter values for NPG = 50000, NSK = 60 and GEN = 600 produced with the MCNP6 were used as in the CE calculations. The only distinct parameters studied here are the SZF and ISN.

Figure 18 below shows a plot of the $k_{inf.}$ versus SZF in a multigroup calculation. It can be seen that the points shown do not differ significantly from each other, with the maximum difference being about 40 pcm. These numbers are about 500 pcm lower than the CE calculation. As such, a 40 pcm variation is insignificant and thus any chosen SZF value is still acceptable. Elaborating further this shows that the spatial mesh error does not compensate for the energy mesh effects. The value of 0.4 was thus assigned.

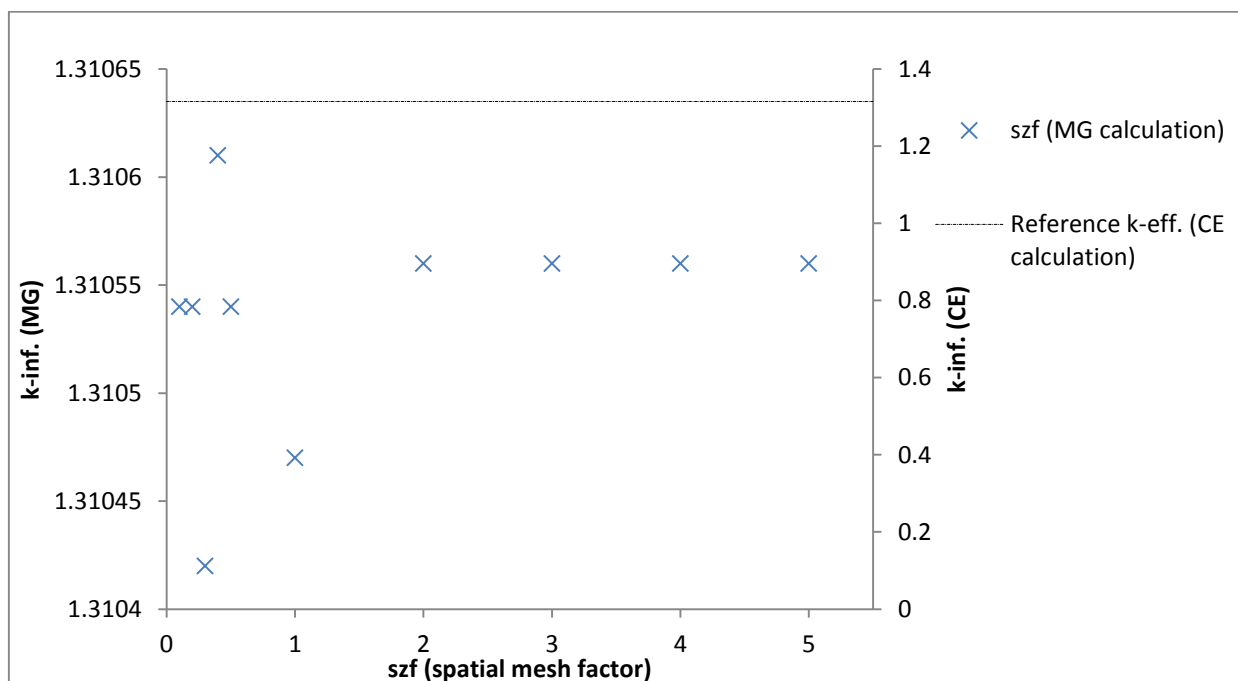


Figure 18 - Plot of $k_{inf.}$ versus SZF in MG calculation.

The ISN value was determined in such a way that simulation converges in terms of the system k_{inf} value. The selected values are 4, 8, 16, 32 and 64. As shown in Figure 19 below, convergence is reached for $ISN = 32$ and $ISN = 64$. It was decided that the value of 32 be used, since this results in a minimized computational time and has shown similar results when the value is set to 64.

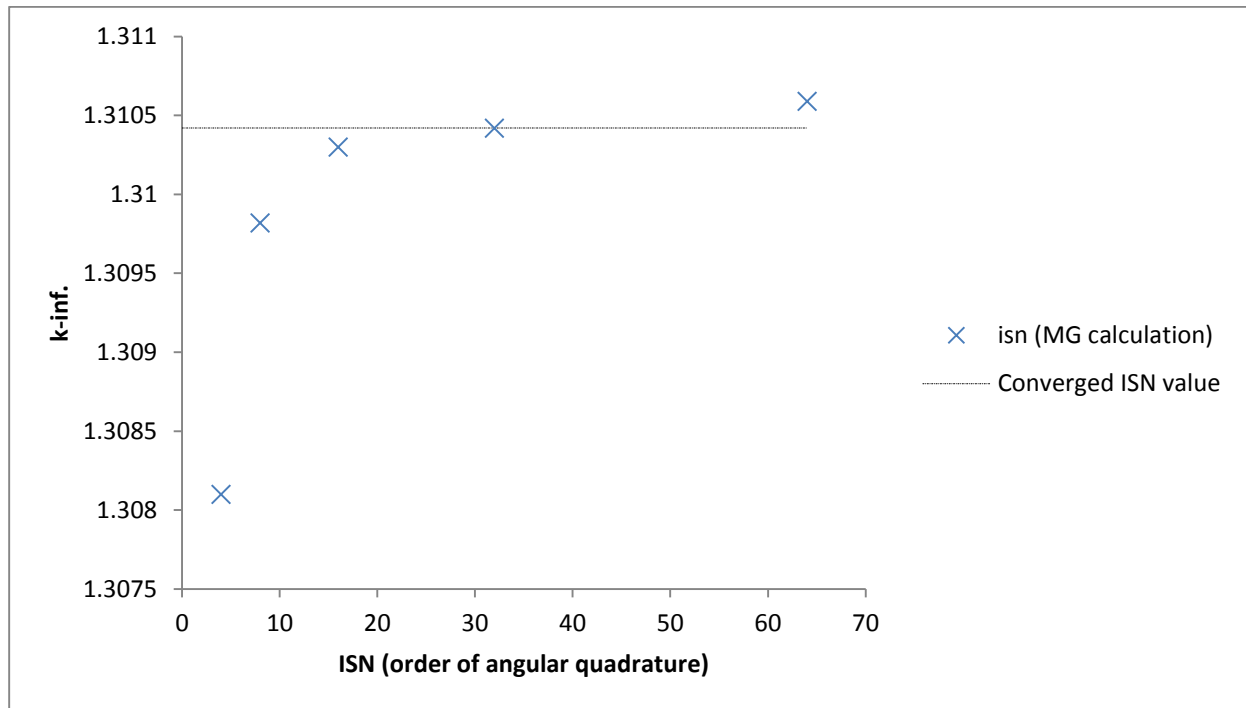


Figure 19 - Convergence of $k_{inf.}$ as function of ISN in MG calculation.

The settings described above were used at CZP and HFP temperature conditions in KENO-VI models for multigroup calculation. It should be noted that these settings are also used in the TSUNAMI-3D models that also use the multigroup energy scheme.

5.3 Base-value calculations

This section presents the base-value results obtained with KENO-VI for the homogeneous, double-heterogeneous and the RPT models of the MHTGR-350 fuel pin cell. Comparisons of the results generated with MG and CE energy schemes are made only for the homogeneous model. In all the models the calculations were performed for CZP and HFP states by solving the forward calculation in KENO-VI.

5.3.1. KENO-VI homogeneous model

Table 13 below shows the multiplication factor values for the KENO-VI homogeneous model. It is observed that the multiplication factor k_{inf} is higher for the CZP state as compared to the HFP in both continuous and multigroup energy calculations. This is due to the Doppler broadening effect shown in Figure 11, as the chances for capture of neutrons that would have otherwise caused fission are increased with increasing temperature. It is observed that the multigroup calculation underestimates the continuous energy calculation by -523 ± 19 pcm and -356 ± 21 pcm at CZP and HFP states, respectively. It should be noted that KENO-VI CE does a Monte Carlo calculation for the pin cell system. However, the KENO-VI MG does the same Monte Carlo calculation but requires the provided multigroup cross-section library and resonance self-shielding cross-sections to be calculated first using a deterministic calculation (see Section 3.6.1). The 238-group cross-section library provided would be prepared for a typical neutron spectrum (and not the exact pin cell spectrum) and differences can therefore be expected. A similar approach is also used in the HELIOS/MASTER calculation described in (Lee, Kim, Cho, Noh, & Lee, 2008). The difference however is that KENO-VI is a Monte Carlo calculation and HELIOS/MASTER uses a transport solver followed by a nodal deterministic solution (Cho, Joo, Cho, & Zee, 2002). An additional group collapsing and homogenization step may also be used. The difference in Lee's work (Lee, Kim, Cho, Noh, & Lee, 2008) between the MCNP calculation and the HELIOS/MASTER calculation was 693 pcm, as was presented in Section 2.7.1.

Table 13 - The multiplication factor results of the homogeneous model.

	Homogeneous	
	CZP	HFP
	$k_{inf.} \pm \sigma$	$k_{inf.} \pm \sigma$
CE calculation (reference)	1.31565 ± 0.00014	1.18661 ± 0.00014
MG calculation	1.31042 ± 0.00013	1.18305 ± 0.00016
Relative difference [pcm]	-523 ± 19	-356 ± 21

The results above are comparable with those found in the benchmark results available (Strydom, Bostelmann, & Yoon, INL/EXT-14-32944 Revision 2, 2015). The same benchmark definitions and cross-section data libraries as used in this study were utilized in this paper. In the paper, CZP state results of the multiplication factor are 1.31576 ± 0.00016 and 1.30897 ± 0.00014 for CE and MG calculations, respectively. The corresponding HFP state the results are 1.18640 ± 0.00016 and 1.18188 ± 0.00014 for CE and MG calculations respectively. The differences

between the two studies for the CE cases are small (<20 pcm) but the differences for the MG calculations are significant (145 and 117 pcm, respectively). Both show the large differences between the CE and MG cases. Possible reasons for these differences with those found in this study arise from the following:

- Both SCALE 6.1 codes are used. An extended version SCALE 6.1.3 is used in this study and in the paper version SCALE 6.1.2 is used.
- The use of different model optimization parameter values. In this study ISN = 32, SZF = 0.4 and SCT = -1. Since none of these are specified in the paper, it is assumed that the default values were rather used.
- In this study, GEN = 600, NPG = 50000 and NSK = 60 whereas in the paper GEN = 500, NPG = 50000 and NSK = 50. A follow-up study should thus be conducted to compare the input decks generated in the current work with those in the paper.

5.3.2 KENO-VI double-heterogeneous model

Table 14 below shows the results obtained in KENO-VI double-heterogeneous model of the fuel pin cell using only the multigroup energy spectrum. A similar trend is observed where, as the temperature increases from CZP to HFP state, the multiplication factor value decreases due to the Doppler broadening effect. The capture cross-sections of ^{238}U nuclei increase as the temperature increases. When comparing the multigroup calculations of the double-heterogeneous and homogeneous models at CZP and HFP states, the multiplication factor values are higher in heterogeneous model approximately by 5640 pcm. A similar result was observed by (Strydom, Bostelmann, & Yoon, INL/EXT-14-32944 Revision 2, 2015) in which the differences amounted to about 6000 pcm. This is because by lumping the fuel (TRISO particles) the resonance escape probability p is increased, which is directly proportional to the multiplication factor. As the name suggests, the resonance escape probability is the probability that the neutron escapes the resonance region as it slows down to lower energies to cause fission.

Table 14 - The multiplication factor results of the double-heterogeneous model.

	Double-heterogeneous	
	CZP	HFP
	$k_{\text{inf.}} \pm \sigma$	$k_{\text{inf.}} \pm \sigma$
Multigroup energy	1.36321 ± 0.00013	1.24315 ± 0.00013

In the paper by (Strydom, Bostelmann, & Yoon, INL/EXT-14-32944 Revision 2, 2015), the same double-heterogeneous model for the MHTGR-350 pin cell was constructed with the same settings as those used for the homogeneous model. The multiplication factor values obtained are 1.36162 ± 0.00015 and 1.24202 ± 0.00013

at CZP and HFP states respectively. The relative differences of these in comparison with those in Table 14 are 159 ± 20 pcm and 113 ± 18 pcm, at CZP and HFP states respectively. These error margins are consistent with those found for the homogeneous model case and this reflects a systematic difference between CZP and HFP calculations. These differences cannot be ascribed to geometric modelling effects since the continuous energy models produced similar trends. The MG treatment in the group collapsing can therefore be assigned as the cause for the differences in results between this study and the benchmark results by (Strydom, Bostelmann, & Yoon, INL/EXT-14-32944 Revision 2, 2015).

5.3.3 The standard RPT model

The results obtained with KENO-VI double-heterogeneous model in Section 5.3.2 are used as reference for all the RPT model results since the RPT models represent an alternative modelling approach that can be adopted when the transport lattice codes are incapable of propagating uncertainties for the double-heterogeneous systems.

The results of the standard RPT model of KENO-VI are shown in Table 15 below. The r_{RPT} value was obtained by interpolation methods such that the condition $|k_{\text{inf.}}(\text{RPT}) - k_{\text{inf.}}(\text{Ref.})| \leq 20$ pcm was met. The r_{RPT} was fairly adjusted and as expected, this radius in all RPT models is smaller than the fuel compact radius of the reference model.

Table 15 - Results of the standard RPT model.

	Standard RPT model	
	CZP	HFP
	$k_{\text{inf.}} \pm \sigma$	$k_{\text{inf.}} \pm \sigma$
Double-heterogeneous MG (reference)	1.36321 ± 0.00013	1.24315 ± 0.00013
RPT radius [cm]	0.40760	0.41413
RPT results	1.36323 ± 0.00015	1.24310 ± 0.00015
Relative difference [pcm]	2 ± 20	-5 ± 20

5.3.4 The modified RPT model

The results obtained with the modified RPT KENO-VI model are shown in Table 16 below.

Table 16 - Results of the modified RPT model.

	Modified RPT	
	CZP	HFP
	$k_{inf.} \pm \sigma$	$k_{inf.} \pm \sigma$
Double-heterogeneous MG (reference)	1.36321 ± 0.00013	1.24315 ± 0.00013
RPT radius [cm]	0.498702	0.508676
RPT results	1.36340 ± 0.00014	1.24318 ± 0.00014
Relative difference [pcm]	19 ± 19	3 ± 19

In all RPT models, it was observed that the adjusted r_{RPT} value for the CZP state cannot be used for the equivalent HFP state since the resulting multiplication factor gives significant relative errors in comparison to the reference HFP state. This means that the r_{RPT} value must be calculated for both temperature states.

The RPT models are verified of their capability to reproduce the reference double-heterogeneous model neutron flux distribution in the next section. Further comparisons for the burnup dependent fuel isotopes and the $k_{inf.}$ at different graphite compact temperatures should be investigated.

5.3.5 Comparisons of the base-value KENO-VI models

In Figure 20-23, the neutron flux distribution was analysed and plotted in all regions at CZP and HFP states across the KENO-VI models of the MHTGR-350 pin cell.

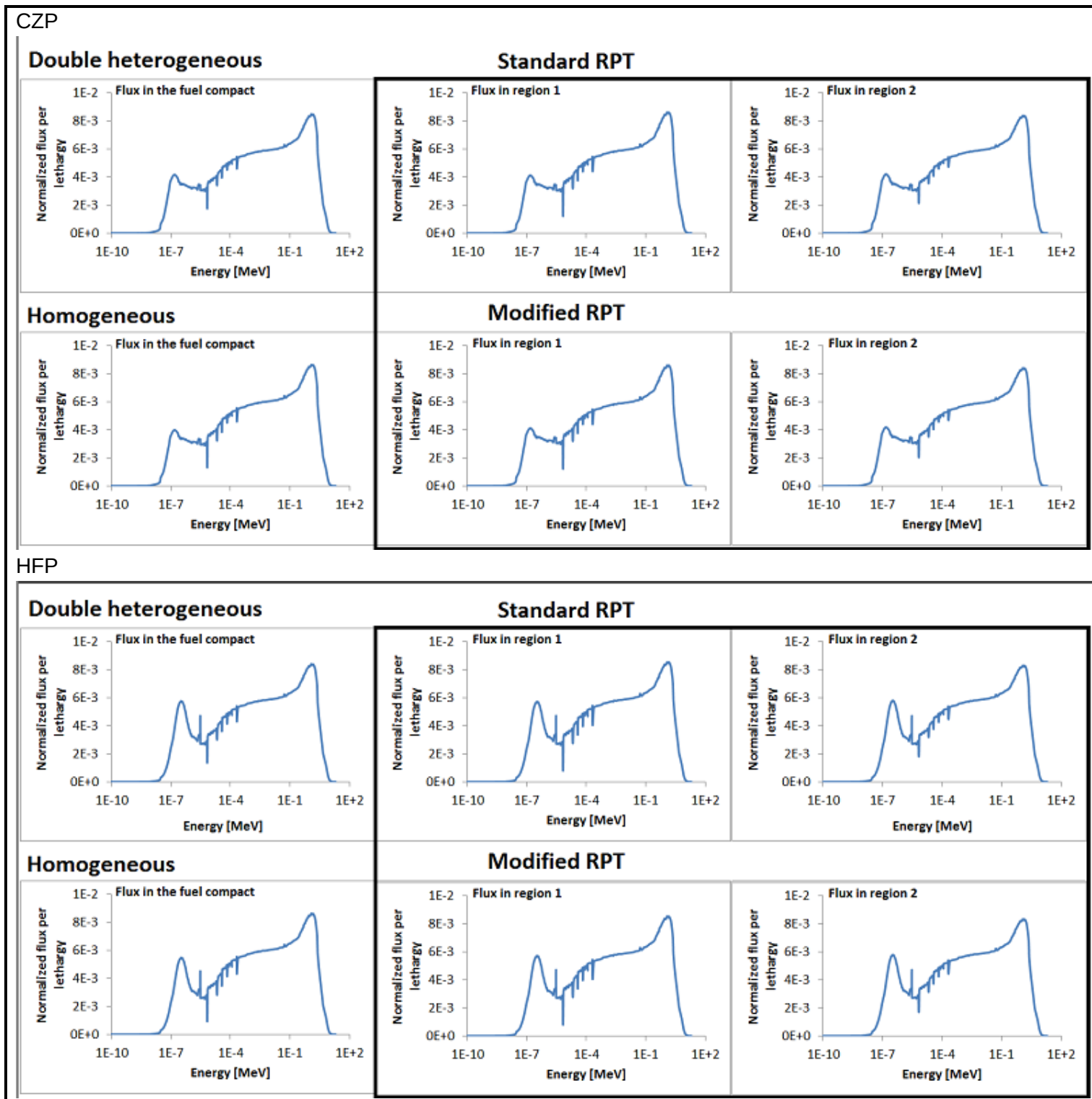
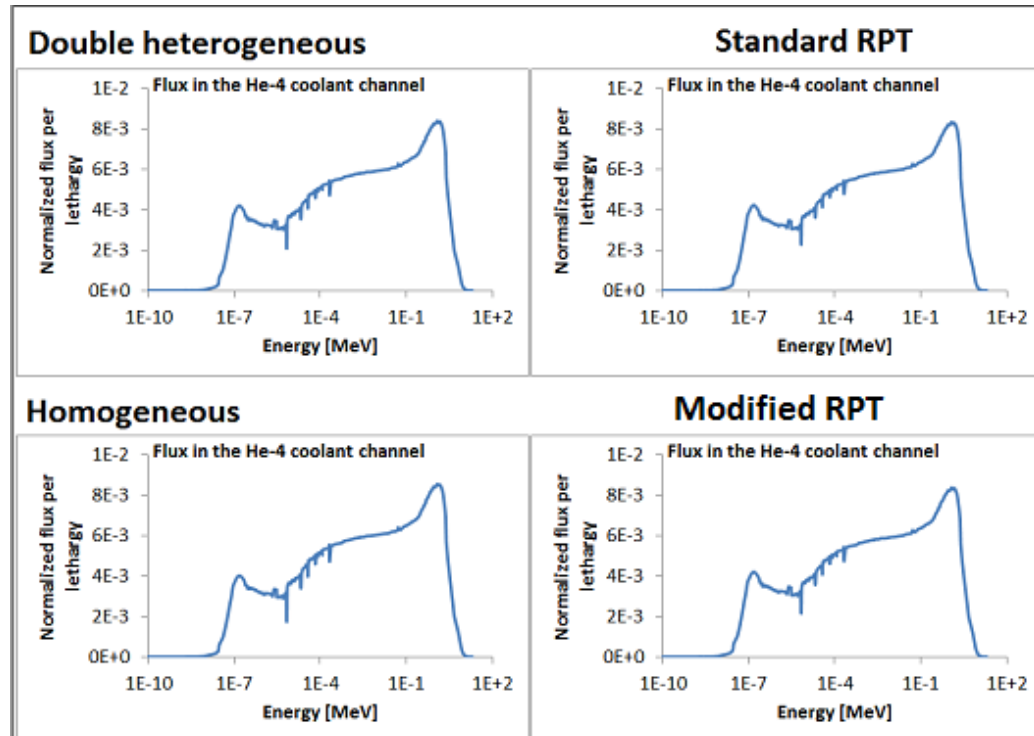


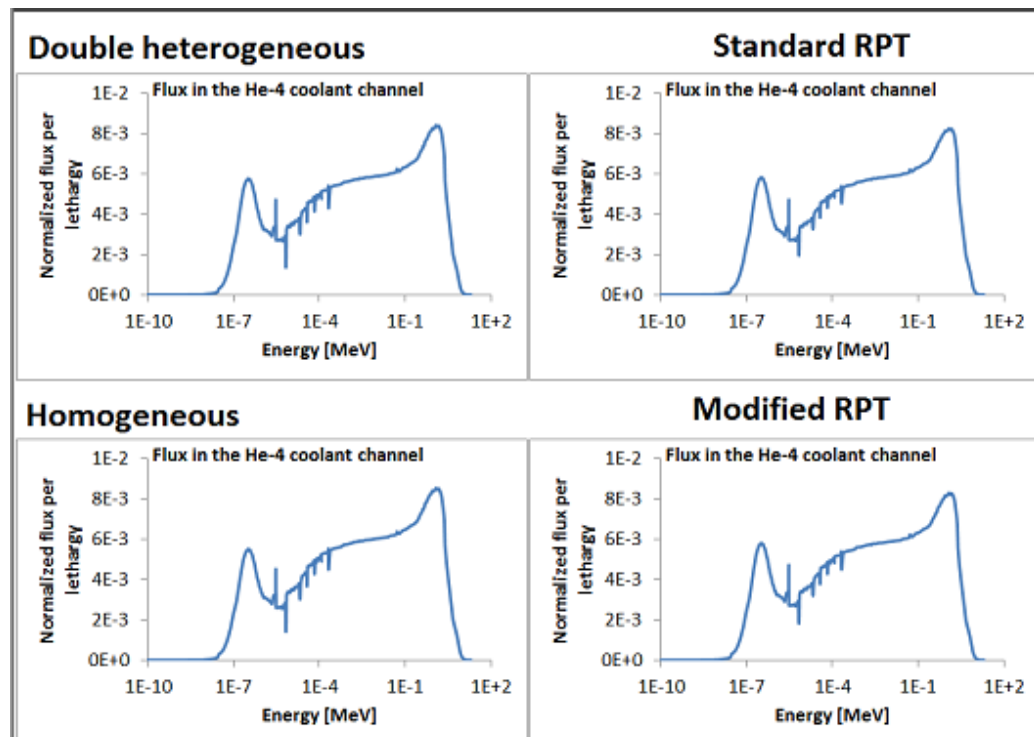
Figure 20 - Normalized flux per lethargy in the compact of the models at CZP and HFP.

It should be noted that in the standard and modified RPT models the fuel compact consists of two regions hence the highlighted sections in Figure 20 above signifies this.

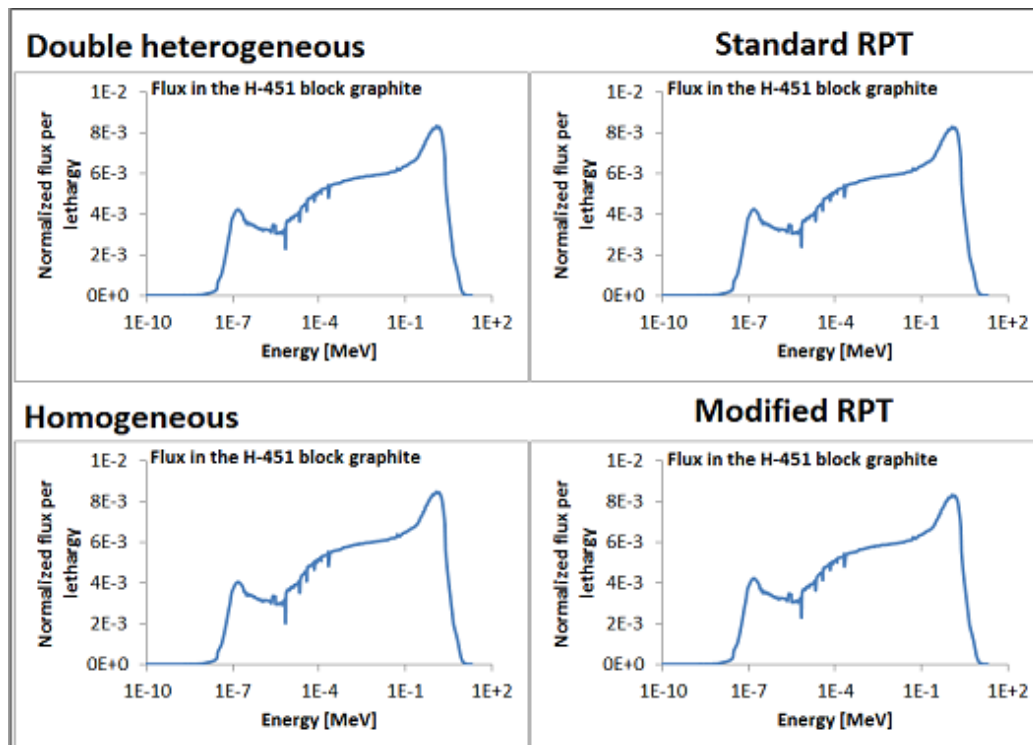
CZP



HFP



CZP



HFP

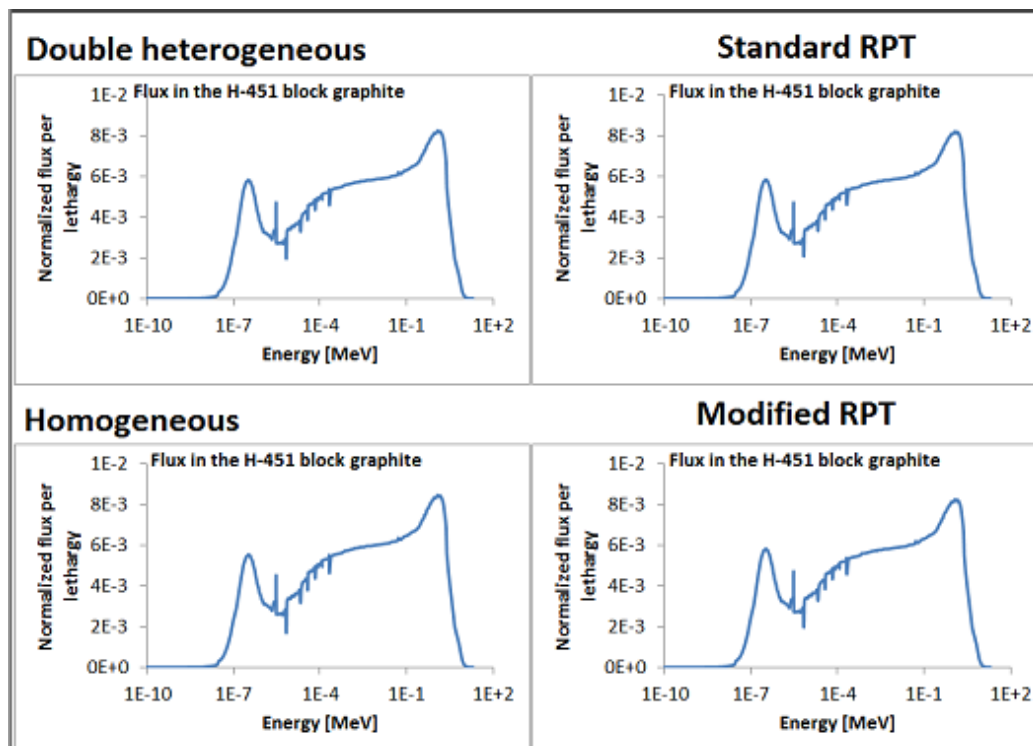
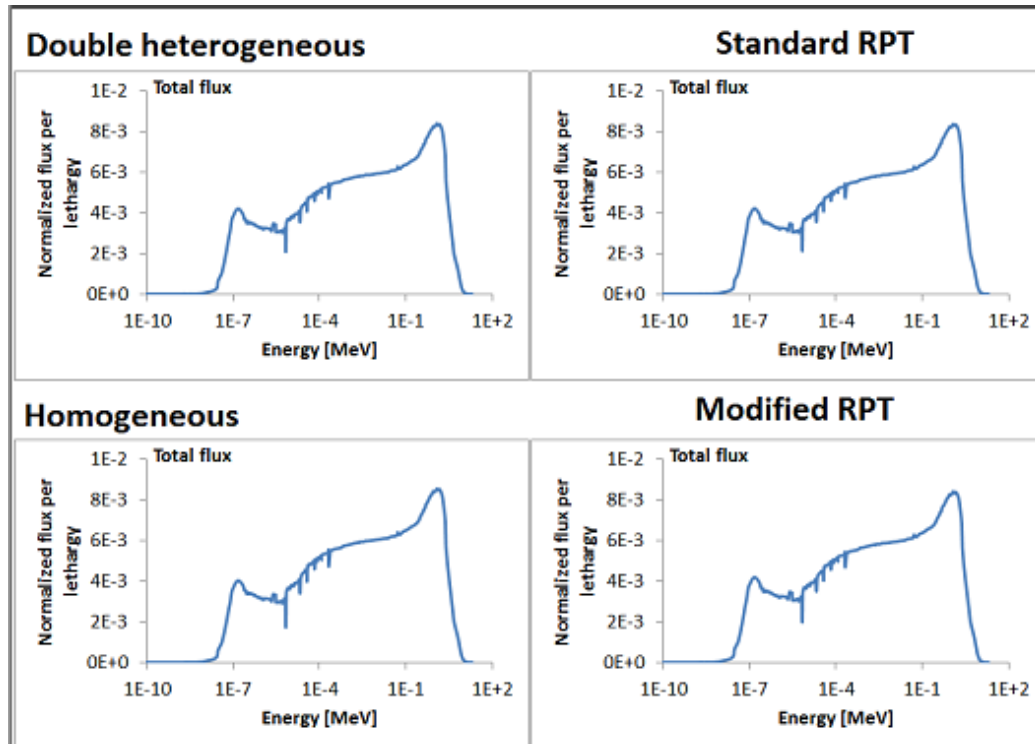


Figure 21 - Normalized flux per lethargy in the graphite block of the models at CZP and HFP.

CZP



HFP

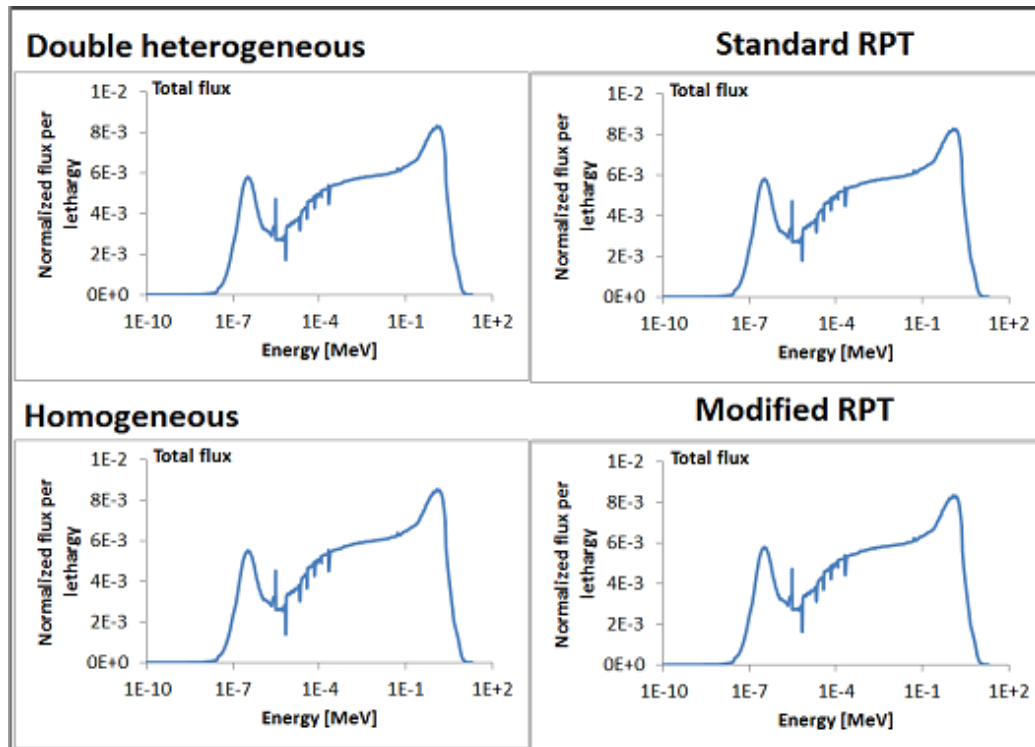
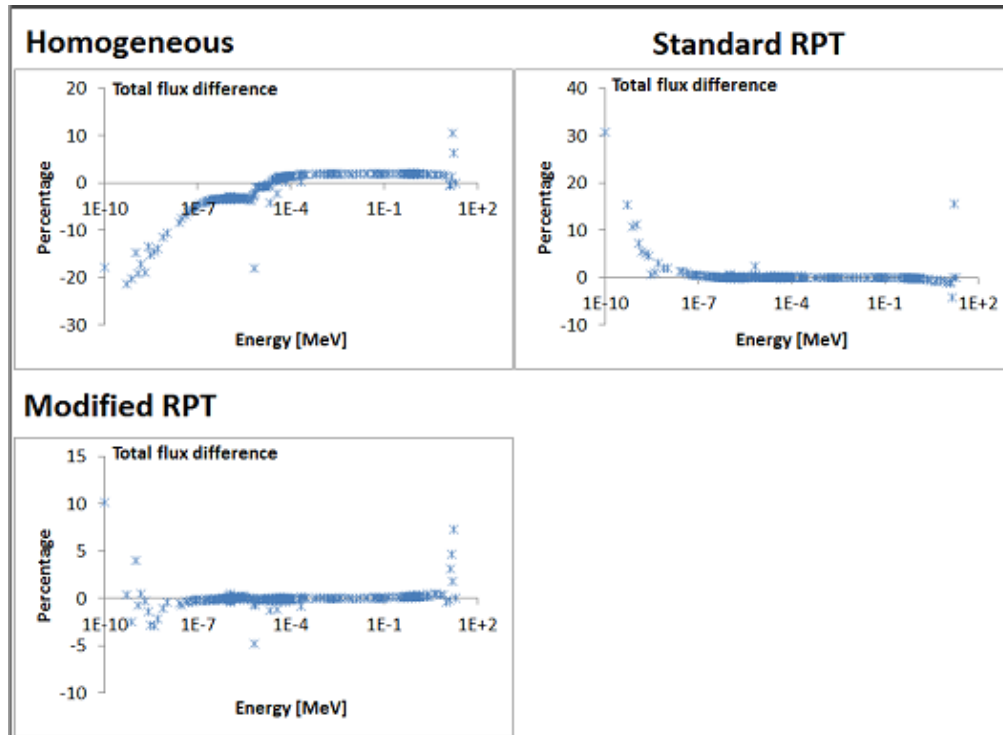


Figure 22 - Sum of all fluxes in the regions of the models at CZP and HFP.

CZP



HFP

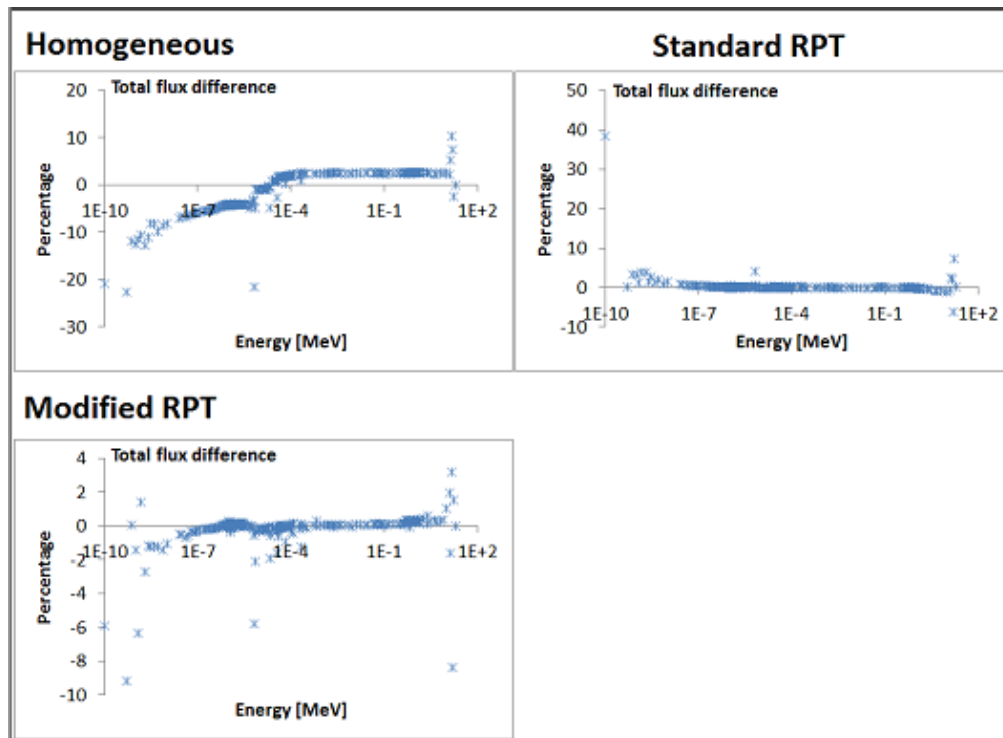


Figure 23 - Percentage flux differences of the models at CZP and HFP.

Figure 20 through Figure 23 above show the normalized flux per lethargy in the regions, the total flux, and the relative total flux differences for all KENO-VI models of the MHTGR-350 fuel pin cell at both the CZP and HFP states. First the neutron fluxes in all regions were divided by lethargy

value and then normalized to one by dividing the result across all energy groups in a region by their sum so as to compare the spectrum. The flux difference in the plots was determined to see the relative difference of the flux in the reference double-heterogeneous model (chosen as a reference) to the respective KENO-VI models.

In the homogeneous model, of the 238 energy groups, 30 energy groups gave relative differences of less than 1% while 178 energy groups gave relative differences between 1 and 4%.

In the standard RPT model, of the 238 energy groups about 217 energy groups gave relative differences of less than 1% while 4 energy groups gave relative differences between 1 and 2%. This already signifies that standard RPT model has a fair approximation of the reference model. In the modified RPT model, of the 238 energy groups about 222 energy groups gave relative differences of less than 1% while 5 energy groups gave relative differences between 1 and 2%. The modified RPT model matches closely the reference double-heterogeneous model through inspection of these numbers.

In all the models, discrepancies were found at both edges of the energy spectrum (very low and very high neutron energies) that gave differences amounting between 10 to 40%. These regions can be of concern when their cross-sections are collapsed, and these cross-sections will need special attention. On the other hand the flux levels and cross-sections at these very high and very low energies may lead to small reaction rates that may make the differences negligible. By studying the reaction rates, the importance can be established. This falls outside the scope of this work.

Since the energies of interest where most of the nuclear reactions in the MHTGR-350 pin cell model occur would not be at the edges of the spectrum, this effect should not lead to rejection of the use of the RPT methodology.

5.4 Uncertainty and sensitivity assessment results

In addition to the base value or nominal case results presented in Section 5.3, this section presents uncertainty and sensitivity results obtained with the TSUNAMI-3D module of the SCALE 6.1 code package. The results from the homogeneous and RPT standard and modified models of MHTGR-350 fuel pin cell at CZP and HFP states, using the 238 multigroup ENDF-B-VII.0 cross-section library are presented. It should be noted that with the current version of SCALE used in this study, propagation of uncertainties and the calculation of sensitivity coefficients could not be carried out on models using continuous energy cross-sections or where the double-heterogeneity was modelled using DOUBLEHET unit cell specification.

TSUNAMI-3D utilizes data from the forward and adjoint solutions of the neutron transport equation to generate sensitivity and uncertainty data. The parameters for the adjoint calculation, as was highlighted in Section 4.5.1 are $AGN = GEN - NSK + ASK = 720$, $ASK = 3 \cdot NSK = 180$ and $APG = 3 \cdot NPG = 150000$

5.4.1 Relative differences in the infinite multiplication factor

The equivalent KENO-VI homogeneous model solutions of the multiplication factor were compared with those obtained with TSUNAMI-3D forward calculation. The relative differences between these are 12 ± 18 pcm and 10 ± 21 pcm in the CZP and HFP states, respectively. This is as expected since both modules use the same transport solution. The differences arise due to the statistical nature of the solution.

Similar findings for the KENO-VI RPT models and their respective TSUNAMI-3D models are shown in Table 17 below and this again shows reasonable agreement between both modules.

Table 17 - Relative multiplication factor differences in KENO-VI and TSUNAMI-3D forward solutions in RPT models.

Model	Relative differences [pcm]	
	CZP	HFP
Standard RPT model	-3 ± 20	-18 ± 21
Modified RPT	6 ± 19	-12 ± 20

Table 18 shows the relative differences in the multiplication factor obtained with the TSUNAMI-3D homogeneous model. Results in the CZP state are reasonable and thus are acceptable. However, in the HFP case the relative differences are quite large. This is most probably because the numbers ascribed for APG and AGN were under-sampled. The use of much larger adjoint parameter values means longer simulation run times and, due to limited amount of time and computational resources, the above results were accepted. It is therefore suggested that for the submission of results by the North West University team to the IAEA CRP coordinator that the adjoint calculations be calculated with generations greater than 6000. This should reduce the errors to the limit required.

Table 18 - Relative difference in the TSUNAMI-3D forward and adjoint multiplication factor for the homogeneous model.

	Homogeneous	
	CZP	HFP
$k_{inf.}$ (forward)	1.31054 ± 0.00013	1.18295 ± 0.00014
$k_{inf.}$ (adjoint)	1.30980 ± 0.00250	1.18020 ± 0.00340
Relative difference [pcm]	-74 ± 250	-275 ± 340

Similar analysis was carried onto the TSUNAMI-3D RPT models which are shown in Table 19 and Table 20. The adjoint control parameters (APG and AGN) should thus be revised using larger samples to minimize such differences with their respective forward solutions.

Table 19 - Relative difference in the TSUNAMI-3D forward and adjoint multiplication factor for the standard RPT model.

	Standard RPT model	
	CZP	HFP
$k_{inf.}$ (forward)	1.36320 ± 0.00013	1.24292 ± 0.00015
$k_{inf.}$ (adjoint)	1.36410 ± 0.00290	1.24350 ± 0.00300
Relative difference [pcm]	90 ± 290	58 ± 300

Table 20 - Relative difference in the TSUNAMI-3D forward and adjoint multiplication factor for the modified RPT model.

	Modified RPT model	
	CZP	HFP
$k_{inf.}$ (forward)	1.36346 ± 0.00013	1.24306 ± 0.00015
$k_{inf.}$ (adjoint)	1.36220 ± 0.00270	1.24740 ± 0.00270
Relative difference [pcm]	126 ± 270	-434 ± 270

5.4.2 The $k_{inf.}$ relative standard deviation due to cross-section covariance data

The relative standard deviation of the infinite multiplication factor $k_{inf.}$ due to cross-section covariance data for the TSUNAMI-3D models is shown in Table 21. This is expressed as $\Delta \pm \sigma$. The delta represents the error due to nuclear covariance data and the sigma is the statistical error. By increasing the control parameters used i.e. the APG, AGN, NPG and GEN in the forward and adjoint calculations, the sigma value will be minimized to the required precision. However, the delta value which is larger than sigma by a factor of a thousand will retain its value with the initial sigma interval of (-0.0001, 0.0001). It can be concluded that the error due to propagated nuclear cross-section covariance is significant and should not be ignored in the uncertainty propagation in the subsequent benchmark exercises.

The RPT models could not be compared with the double-heterogeneous model since the latter model cannot be propagated in terms of uncertainties directly using the current version of SCALE 6.1. A suggestion is that the lattice model that explicitly defines TRISO particles that are uniformly distributed in the compact can be established in KENO-VI and analysed and then the RPT models can be compared with the lattice model. It is thus recommended in future work that the lattice model be built to further justify the use of the RPT model in uncertainty propagation.

Table 21 - Relative standard deviation of k_{inf} . due to cross-section covariance data.

	Relative standard deviation [% $\Delta k/k$]	
	CZP	HFP
Homogeneous	0.5222 ± 0.0001	0.5734 ± 0.0001
Standard RPT model	0.5032 ± 0.0001	0.5451 ± 0.0001
Modified RPT	0.5034 ± 0.0001	0.5440 ± 0.0002

Similar results to those of the homogeneous case shown in Table 21 were observed in the report paper by (Reitsma , Strydom, Bostelmann, & Ivanov, 2014) for a similar homogeneous model with the relative standard deviation of 0.5409 ± 0.0002 and 0.5707 ± 0.0002 at CZP and HFP states respectively.

5.4.3 The top five neutron-nuclide contributors to k_{inf} . uncertainty

The types of nuclear reactions that significantly impact on the uncertainty in the multiplication factor of the MHTGR-350 fuel pin cell are addressed in the following.

Table 22 below shows the uncertainty contribution to k_{inf} for the top five reaction pairs in the CZP and HFP states, respectively. These were calculated for all TSUNAMI-3D models.

Table 22 - The top five nuclear reaction contributors to the uncertainty in k_{inf} at CZP.

Rank	Reaction	Contribution to uncertainty in k_{inf} . [% $\Delta k/k$]
Homogeneous		
1	$^{238}\text{U} (n, \gamma) - ^{238}\text{U} (n, \gamma)$	0.3222
2	$^{235}\text{U} (\bar{\nu}) - ^{235}\text{U} (\bar{\nu})$	0.2654
3	$^{235}\text{U} (n, \gamma) - ^{235}\text{U} (n, \gamma)$	0.2594
4	$^{238}\text{U} (n, n) - ^{238}\text{U} (n, n)$	0.1050
5	$^{235}\text{U} (n, f) - ^{238}\text{U} (n, \gamma)$	0.0976
Standard RPT		
1	$^{238}\text{U} (n, \gamma) - ^{238}\text{U} (n, \gamma)$	0.2852
2	$^{235}\text{U} (\bar{\nu}) - ^{235}\text{U} (\bar{\nu})$	0.2669
3	$^{235}\text{U} (n, \gamma) - ^{235}\text{U} (n, \gamma)$	0.2602
4	C-graphite (n, n) - C-graphite (n, n)	0.1000
5	$^{235}\text{U} (n, f) - ^{235}\text{U} (n, \gamma)$	0.0975
Modified RPT		
1	$^{238}\text{U} (n, \gamma) - ^{238}\text{U} (n, \gamma)$	0.2852
2	$^{235}\text{U} (\bar{\nu}) - ^{235}\text{U} (\bar{\nu})$	0.2669
3	$^{235}\text{U} (n, \gamma) - ^{235}\text{U} (n, \gamma)$	0.2605
4	C-graphite (n, n) - C-graphite (n, n)	0.1003
5	$^{235}\text{U} (n, f) - ^{235}\text{U} (n, \gamma)$	0.0974

In the HFP state, the ranks of neutron nuclide reactions in each model are the same as those highlighted in Table 22. However, the last two contributing reactions to k_{inf} uncertainty are switched and these are not significant in terms of strength.

It can be seen in Table 22 that the capture of a neutron by a ^{238}U isotope and release of gamma ray energy is the main contributor to the uncertainty in the infinite multiplication factor of the MHTGR-350 pin cell in all the models. The second largest contributor to k_{inf} uncertainty is the absorption of neutrons by ^{235}U isotopes which then yields an average number of neutrons when it fissions i.e. $^{235}\text{U} (\bar{\nu})$.

5.4.4 Sensitivity data plots

It has been addressed in Section 3.7 that nuclear reactions that contribute to the sensitivity in the k_{inf} are ranked by use of sensitivity coefficients, which are the implicit and explicit sensitivity coefficients. Table 23 below shows the sensitivity coefficients for the nuclide and reaction type for

the top five contributors in all models. The results show the percentage change in k_{inf} . (i.e. the sensitivity column) that one would observe when the cross-section for each nuclide reaction is increased by 1% uniformly across all the 238 energy groups.

Table 23 - The sensitivity coefficients for each nuclide and reaction type at CZP.

Nuclide	Reaction/contributor	Explicit [%]	Implicit [%]	Sensitivity [%]
Homogeneous				
^{235}U	$\bar{\nu}$	0.9933	0.0000	0.9933
^{235}U	(n, f)	0.2326	-0.0001	0.2325
C-graphite	(n, n')	0.2238	-0.0564	0.1673
C-graphite	(n, n)	0.2234	-0.0564	0.1669
C-graphite	total	0.2162	-0.0564	0.1597
Standard RPT model				
^{235}U	$\bar{\nu}$	0.9934	0.0000	0.9934
^{235}U	(n, f)	0.2269	0.0000	0.2269
C-graphite	(n, n')	0.2422	-0.0443	0.1979
C-graphite	(n, n)	0.2418	-0.0443	0.1975
C-graphite	total	0.2345	-0.0443	0.1901
Modified RPT				
^{235}U	$\bar{\nu}$	0.9934	0.0000	0.9934
^{235}U	(n, f)	0.2260	0.0000	0.2259
C-graphite	(n, n')	0.2429	-0.0441	0.1987
C-graphite	(n, n)	0.2424	-0.0441	0.1983
C-graphite	total	0.2351	-0.0441	0.1909

In the following, plots of sensitivity profiles for the reactions of interest taking place in the MHTGR-350 pin cell are shown. The plots were extracted from the modified RPT model (at CZP). This is because the modified RPT methods have proven to closely reproduce characteristics of a reference double-heterogeneous model in terms of the neutron flux as can be seen in Figure 23. The sensitivity profiles are plotted following the reactions of interest which include ^{238}U (n, γ), ^{235}U ($\bar{\nu}$), ^{235}U (n, γ), C-graphite (n, n), ^{16}O (n, n), ^{29}Si (n, n) and ^4He (n, n) as follows:

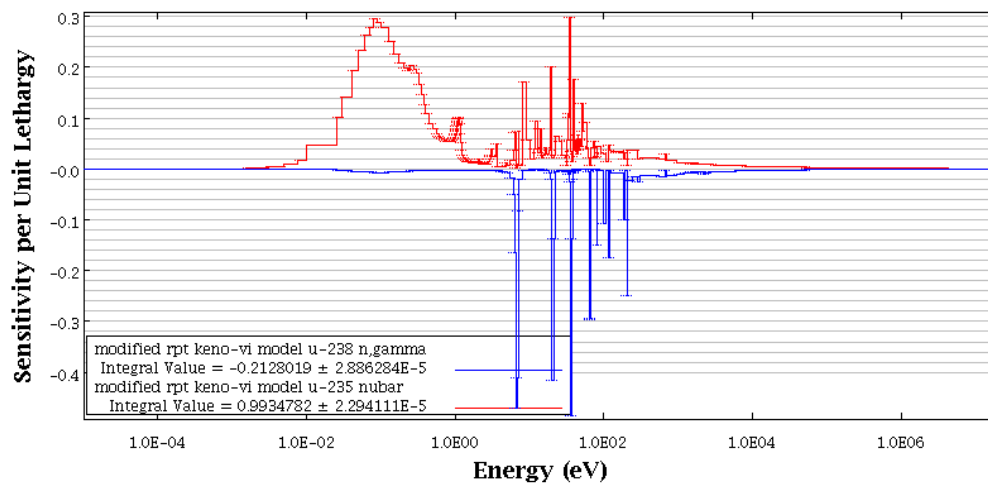


Figure 24 - Sensitivity data plot of ^{238}U (n, γ) and ^{235}U ($\bar{\nu}$) reactions.

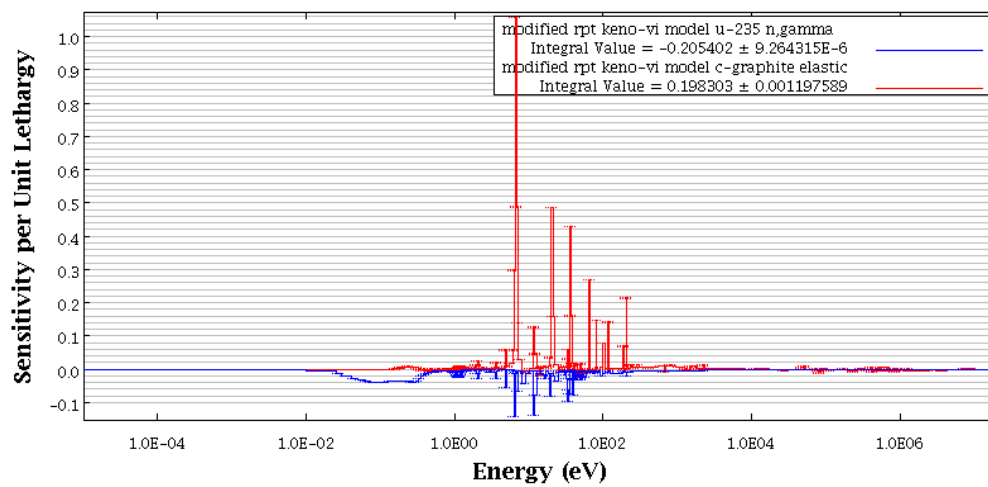


Figure 25 - Sensitivity data plot of ^{235}U (n, γ) and C-graphite (n, n) reactions.

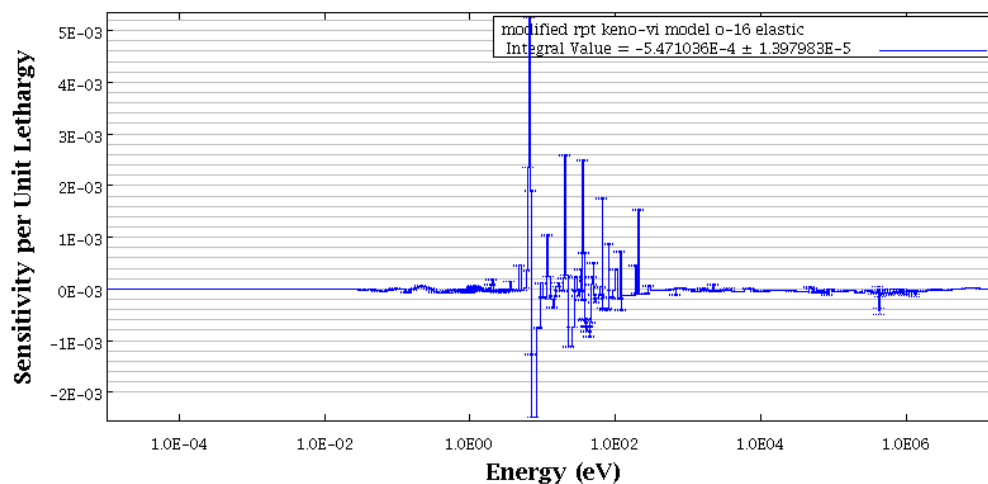


Figure 26 - Sensitivity data plot of ^{16}O (n, n) reaction.

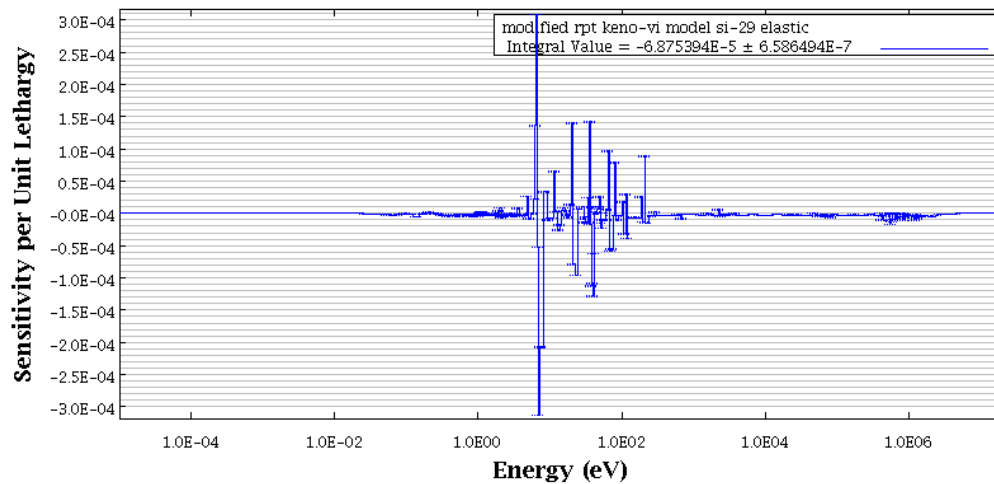


Figure 27 - Sensitivity data plot of ^{29}Si (n, n) reaction.

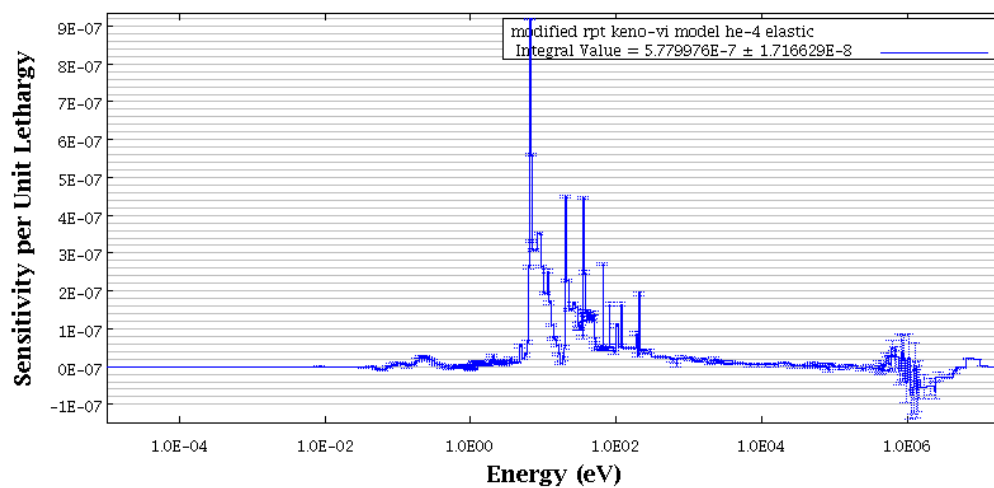


Figure 28 - Sensitivity data plot of the ^4He (n, n) reaction.

The information shown in the legends of the above figures represents a percentage change in the system k_{inf} when the cross-section for the nuclide reaction is increased by 1% uniformly across all the 238 energy groups. For instance, in Figure 24 when the ^{238}U (n, γ) reaction cross-section is increased uniformly by 1% the k_{inf} will decrease (hence the negative sign) by an amount of 0.2128%.

It is observed that there are distinct peaks in the sensitivity plots at specific energies. This means that in calculating the group constants in the latter exercises of the benchmark the group structure should be investigated. Groups should be considered that isolate these peaks, and the effects on the uncertainty should be studied. It is possible that the definition of the group boundaries could influence the outcome of the uncertainty calculated.

5.5 Verification of the KENO-VI and TSUNAMI-3D models

During the course of this study, steps were taken to check that the solutions given by KENO-VI and TSUNAMI-3D models were implemented accurately. These steps are summarised below:

- All model specifications were written using a basic text file editor and the simulation was executed in the Windows command prompt. In a similar way, a tool GeeWiz was used in parallel to create the models and perform the calculations. The solutions generated by GeeWiz and those from executing the text files editor were compared and found to agree with at-least six decimal places.
- The geometric shapes and dimensions specified in the inputs were checked that they resemble those specified in the benchmark by visualization in KENO3D and that these were properly drawn to good scale (as can be seen in Figure 14). Since the capability of KENO3D for automatic generation of volumes in each region of the pin cell was utilized, confirmation was made that these were correct by comparing them with those calculated analytically in Chapter 4.
- A study of the behaviour of the k_{inf} due to temperature change was conducted and this showed the expectations that are bound to happen in support of the theory i.e. as the temperature is increased the k_{inf} decreased and this is in full agreement with the theory presented for Doppler resonance broadening in Chapter 3.
- All the KENO-VI and TSUNAMI-3D models were compared with those of another member in the School team. The solutions of important parameters such as fission density, neutron flux and criticality were in good agreement within at-least four decimal places.

CHAPTER 6 – CONCLUSIONS AND FUTURE RECOMMENDATIONS

6.1 Conclusions

This work covers a portion of the benchmark activity launched by the IAEA CRP for the development of uncertainty treatment methodology specifically for the HTGR reactor type. The reference design used in this study is the MHTGR-350 reactor and focuses specifically on the Reactor physics calculations. Exercises 1a and 1b defined under Phase 1 of the IAEA CRP on HTGR Uncertainties were extracted to perform this study.

These exercises required the modelling of the MHTGR-350 fuel pin cell for the derivation of the microscopic cross-section sets which were then propagated to finding the response parameter called the multiplication factor. The sensitivity of the response due to the variation in the cross-section values were investigated together with its uncertainty. Definitive steps were performed to carry out this analysis and these are described in the paragraphs that follow.

The MHTGR-350 fuel pin cell models were successfully built using the KENO-VI and TSUNAMI-3D modules of the SCALE 6.1 code package. These models were verified following the procedures shown in Section 5.5 and investigations were then carried out.

The MHTGR-350 pin cell was built as homogeneous and double-heterogeneous models that only varied in their fuel regions. The homogeneous model specifies the smeared-out TRISO particles, together with the graphite matrix. The double-heterogeneous model specifies explicitly the TRISO particles for the investigation of their resonance self-shielding effects on the multigroup parameters of interest. Due to limitations of the transport lattice codes for the accurate modelling of the uncertainty propagation in the double-heterogeneous model, the RPT methodology was adopted in this study. The RPT methodology therefore made it possible for the sensitivity and uncertainty analysis through the TSUNAMI-3D module of SCALE 6.1. The double-heterogeneous model could not be used for uncertainty propagation with the version of SCALE 6.1 which was used in this study. In all these models, the ENDF-B-VII.0 cross-section library was used. The multigroup calculations were performed for all the models while continuous energy calculations were performed only in the homogeneous model. As it has previously been said, the current version of SCALE 6.1 used in this study only allows calculations of the double-heterogeneous KENO-VI model using the multigroup energy. In the homogeneous KENO-VI model of the MHTGR-350 pin cell, it was found that MG calculations of the infinite multiplication factor underestimates the results found with CE calculations. This is attributed to the KENO-VI CE calculation performing a Monte Carlo calculation for the fuel pin cell, while KENO-VI MG does the

same Monte Carlo calculation but requires provision of the multigroup cross-section library and resonance self-shielding cross-sections to be calculated first utilizing a deterministic calculation.

The effect of homogenizing the fuel compact in the homogeneous model was found to be underestimating the infinite multiplication factor of the reference double-heterogeneous models, which is the effect observed in many literature studies. The increased multiplication factor of the reference double-heterogeneous models is expected due to the increased resonance escape probability, as it has been noted in Section 5.3.2. (Reitsma , Strydom, Bostelmann, & Ivanov, 2014) assigned the same reasoning to the results acquired for their homogeneous and double-heterogeneous calculations.

Increasing the temperature from CZP to HFP has a major effect in decreasing k_{inf} due to the phenomenon of the Doppler resonance broadening, which influences the cross-sections of the reactions. This effect was observed in all the models and this can be used as part of the verification of the models developed.

Following the base-value calculations, the uncertainty assessment of the results was performed. Since the double-heterogeneous model could not be propagated in terms of uncertainties with the current SCALE 6.1 code, the RPT approach for representation of this model was investigated. Two models were built using the RPT approach. The extent to how well these RPT models represent the reference heterogeneous model was ranked based on the generation of the neutron flux distribution (at least on this level). The neutron flux distribution was determined for the double heterogeneous model in base-value calculations.

It was found that the modified RPT model successfully reproduced the neutron flux distribution of the double-heterogeneous model. This finding is justified by the total flux differences (expressed as percentage) between the reference double-heterogeneous model and the modified RPT model, in which out of the 238 energy groups, about 222 energy groups gave relative differences of less than 1% while 5 energy groups gave relative differences between 1 and 2%. Total flux differences with regard to the homogeneous and standard RPT models are more pronounced in contrast to the modified RPT model. Thus, as an alternative to modelling double-heterogeneous systems presented by most HTGR reactor concepts, the transport lattice codes can adopt a modified RPT methodology for a more accurate representation.

Under the uncertainty analysis, the relative differences between forward and adjoint calculation of the multiplication factor were, on the overall, found to be larger. This was attributed to the use of under-sampled values for the adjoint parameters to which their increase would facilitate the convergence of the forward and adjoint solutions. Larger adjoint parameter values would imply longer simulation run times and due to time constraints framed within this project, these results

were accepted. A directive is that for the submission of results by the North West University team to the IAEA CRP coordinator, larger adjoint parameter values should be used.

The relative standard deviation for the infinite multiplication factor due to cross-section covariance data were found be larger and thus should not be ignored in the uncertainty propagation of subsequent benchmark exercises. The sigma value could be minimized to the required precision by increasing the control parameter values. For a fair comparison of results found with RPT models in terms of uncertainty propagation, a lattice model of the coated particles is suggested since the double-heterogeneous model cannot be used for uncertainty propagation with the version of SCALE used in this study.

The major neutron-nuclide contributors to the uncertainty in the infinite multiplication were found to be ^{238}U (n, γ) and ^{235}U ($\bar{\nu}$) reactions, as can be seen in Table 22. The sensitivity profiles of the infinite multiplication factor due to a uniform increase of the reaction cross-sections were generated, and it was found that $k_{\text{inf.}}$ was highly sensitive to $^{235}\text{U}(\bar{\nu})$ and $^{235}\text{U}(\text{n,f})$ reactions.

In terms of contributing to the IAEA CRP on HTGR UAM to address nuclear covariance data provided by Nuclear Data Organizations, it was found that the contribution from the nuclear covariance data was significant in terms of the propagation of the uncertainty in $k_{\text{inf.}}$.

6.2 Recommendations for future research

A list of recommended actions aimed at facilitating and supplementing the current study is as follows:

- Monitoring convergence studies of the Shannon entropy of the fission source and multiplication factor is important in Monte Carlo methods. A built-in function for generation of Shannon entropy of the fission source should be incorporated in KENO-VI code. Thus this point is raised for the KENO-VI code developers.
- A DOUBLEHET unit cell specification capability should be made available in TSUNAMI-3D module for accurate modelling and propagation of uncertainties of double-heterogeneous problems for comparison with the RPT models. However, it is believed that this is currently being done.
- Prior to using the RPT approach to propagating uncertainties for double-heterogeneous systems, the results for the pin cell must be tested against a cell model based on a lattice of the coated particles.
- Before presenting results to the IAEA CRP coordinator, the calculations must be repeated in which the number of generations for the adjoint calculations must be increased so that the statistical error in $k_{\text{inf.}}$ can be of the order of 15 pcm.

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APPENDIX A

A1. The KENO-VI and TSUNAMI-3D model input files

The input files for the KENO-VI and TSUNAMI-3D models can be constructed and edited by use of the basic text editors. In this study, the text editor was used and, for purposes of verification of results and obtaining 3D visual images generated by KENO3D of the MHTGR-350 pin cell, some of the inputs were specified and run in the SCALE 6.1 GeeWiz interface.

The layout of the input files are given in the following using as an example the homogeneous model specifications of the pin cell. It should be noted that line numbers are not part of the model and are included here for referencing in discussions:

The KENO-VI input file for the homogeneous model:

Line Number	Input File
1	=csas6
2	The homogeneous KENO-VI model of the MHTGR-350 fuel pin cell.
3	v7-238
4	read composition
5	u-235 1 0 0.00015765 293 end
6	u-238 1 0 0.00084864 293 end
7	o-16 1 0 0.0015094 293 end
8	c-graphite 1 0 0.069958 293 end
9	si-28 1 0 0.0028457 293 end
10	si-29 1 0 0.00014456 293 end
11	si-30 1 0 9.5408e-05 293 end
12	he-4 2 0 2.46e-05 293 end
13	c-graphite 3 0 0.092756 293 end
14	end composition
15	read celldata
16	latticecell trianpitch fuelr=0.6225 1 gapr=0.635 2 hpitch=0.9398 3 end
17	centrmdata
18	isn=32
19	end centrmdata
20	moredata
21	szf=0.4
22	end moredata
23	end celldata
24	read parameter
25	npg=50000
26	nsk=60
27	gen=600
28	sig=0.00014

29	flx=yes
30	fdn=yes
31	htm=yes
32	nub=yes
33	pmv=yes
34	far=yes
35	gas=yes
36	cds=yes
37	mfx=yes
38	pms=yes
39	end parameter
40	read mixt
41	sct=-1
42	end mixt
43	read geometry
44	global unit 1
45	com="The MHTGR-350 fuel pin cell"
46	cylinder 1 0.6225 2.464 -2.464
47	cylinder 2 0.635 2.464 -2.464
48	rhexprism 3 0.9398 2.464 -2.464
49	media 1 1 1 vol=5.999282
50	media 2 1 2 -1 vol=0.243354
51	media 3 1 3 -2 vol=8.834963
52	boundary 3
53	end geometry
54	read bounds
55	body=3
56	all=reflected
57	end bounds
58	read gridgeometry 1
59	tolerance=1e-006
60	xlinear 20 -1.08519 1.08519
61	tolerance=1e-006
62	ylinear 20 -0.9398 0.9398
63	tolerance=1e-006
64	zlinear 5 -2.464 2.464
65	end gridgeometry
66	end data
67	end

The TSUNAMI-3D input file for the homogeneous model:

Line Number	Input File
1	=tsunami-3d-k6
2	The homogeneous TSUNAMI-3D model of the MHTGR-350 fuel pin cell.
3	v7-238
4	read composition
5	u-235 1 0 0.00015765 293 end
6	u-238 1 0 0.00084864 293 end
7	o-16 1 0 0.0015094 293 end
8	c-graphite 1 0 0.069958 293 end
9	si-28 1 0 0.0028457 293 end
10	si-29 1 0 0.00014456 293 end
11	si-30 1 0 9.5408e-05 293 end
12	he-4 10 0 2.46e-05 293 end
13	c-graphite 11 0 0.092756 293 end
14	end composition
15	read celldata
16	latticecell triangpitch fuelr=0.6225 1 gapr=0.635 10 hpitch=0.9398 11 end
17	more data szf=0.4 end more
18	centrm data isn=32 end centrm
19	end celldata
20	read parameter
21	gen=600
22	npg=50000
23	nsk=60
24	agn=1800
25	apg=150000
26	ask=180
27	flx=yes
28	fdn=yes
29	htm=yes
30	nub=yes
31	pmv=yes
32	far=yes
33	gas=yes
34	cds=yes
35	mfx=yes
36	pms=yes
37	end parameter
38	read mixt
39	sct=-1
40	end mixt
41	read geometry
42	global unit 1
43	com="The MHTGR-350 fuel pin cell"

44	cylinder 1 0.6225 2.464 -2.464
45	cylinder 2 0.635 2.464 -2.464
46	rhexpism 3 0.9398 2.464 -2.464
47	media 1 1 1 vol=5.999282
48	media 10 1 2 -1 vol=0.243354
49	media 11 1 3 -2 vol=8.834963
50	boundary 3
51	end geometry
52	read bounds
53	body=3
54	all=reflected
55	end bounds
56	read gridgeometry 1
57	tolerance=1e-006
58	xlinear 20 -1.08519 1.08519
59	tolerance=1e-006
60	ylinear 20 -0.9398 0.9398
61	tolerance=1e-006
62	zlinear 5 -2.464 2.464
63	end gridgeometry
64	end data
65	read sams
66	makeimp
67	pltp
68	prtgeom
69	prtimp
70	usemom
71	end sams
72	end

A2. Sensitivity data plots

The sensitivity data file (SDF extension) that is available for plotting is stored in the same directory as the input file when the simulation completes (together with other text and HTML-formatted output files). These are given for all reaction types in all regions. The following are the steps followed for obtaining the plots of sensitivity data:

- Open the Javapeño-3D applet in the C:\scale6.1\javapeno path directory.
- A new window will appear above the monitor screen which have the File, Options, Format, Window and Help tabs.
- Click on the File tab. Various options are available in the File tab and for our aim in this section, the Open Dataset option was selected. A new window appears.
- In the window, navigate to the path directory where the input file of the model is stored. In this directory, output files are available and of our interest is the SDF file extension.
- Double-clicking on the SDF file displays the window having the sensitivity information available for plotting on the far right corner of the monitor screen.
- Finally select the reaction type of interest. The sensitivity data plot for this type will automatically appear which can then be captured using the snipping tool functionality within Windows 7.

A3. Generation of KENO3D images

KENO3D allows for visualization of 3D images that are specified for input models in KENO-VI and KENO V.a modules of SCALE 6.1. The input models can be built either using a basic text file editor or using GeeWiz functionality. The 3D images can be generated readily when using GeeWiz i.e. by clicking on Keno3D icon above the monitor screen, which can then be captured using the snipping tool.

When a general text file editor is used instead, first the model input files need to be opened via GeeWiz as follows:

- Open GeeWiz programme by clicking on Windows start button and looking for this item.
- When the programme loads click on File tab. From here follow the path directory of the model input file and click on it.
- The model specifications in the text file editor will automatically be written in the GeeWiz programme. The Keno3D icon will also be visible which can now be clicked for 3D visual of the input model and captured using the snipping tool.

KENO3D allows for rotation of 3D model images, zooming, selection and display of certain model parts, cut-away views and editing colours which are displayed in the legends.