AUTOMATED SPECTRAL ZONES SELECTION METHODOLOGY FOR
DIFFUSION THEORY DATA PREPARATION FOR PEBBLE BED REACTOR
ANALYSIS

A Dissertation in
Nuclear Engineering

by
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ABSTRACT

A methodology is developed for the determination of the optimum spectral zones in Pebble Bed Reactors (PBR). In this work a spectral zone is defined as a zone made up of a number of nodes whose characteristics are collectively similar and that are assigned the same few-group diffusion constants. In other words the spectral zones are the regions over which the few-group diffusion parameters are generated.

The identification of spectral boundaries is treated as an optimization problem. It is solved by systematically and simultaneously repositioning all zone boundaries to achieve the global minimum error between the reference transport solution (MCNP) and the diffusion code solution (NEM). The objective function for the optimization algorithm is the total reaction rate error, which is defined as the sum of the leakage, absorption and fission reaction rates error in each zone. An iterative determination of group-dependent bucklings is incorporated into the methodology to properly account for spectral effects of neighboring zones. A preferred energy group structure has also been chosen.

This optimization approach with the reference transport solution has proved to be accurate and consistent, however the computational effort required to complete the optimization process is significant. Thus a more practical methodology is also developed for the determination of the spectral zones in PBRs. The reactor physics characteristics of the spectral zones have been studied to understand the nature of the spectral zone boundaries. The practical tool involves the use of spectral indices based on few-group diffusion theory whole core calculations. With this methodology, there is no need to first have a reference transport solution. It is shown that the diffusion-theory coarse group
fluxes and the effective multiplication factor computed using zones based on the practical index agrees within a narrow tolerance with those of the reference approach. Therefore the “practical” index provides a convenient method for the determination of spectral zones without the recourse to a reference transport solution.

The use of the optimum spectral boundaries together with the preferred energy group structure renders the NEM code a practical tool for analyzing the PBR core.
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Chapter 1

Introduction

1.1 High Temperature Gas-Cooled Reactor of PBMR Type

Recent indications of growing power needs and possibilities of future power shortages in the United States, South Africa and other parts of the world have driven the interest in increasing power generation capabilities. In particular, the nuclear power generation industry has taken a new turn and the building of new nuclear power reactors is a top item on the agenda of nuclear engineers, scientists and researchers, and politicians.

A few countries are involved in the forum on the development of the Next Generation Nuclear Energy Systems. The purpose is to develop an advanced nuclear power reactor that has the following qualities: proliferation-resistant, sustainable, safe, reliable, and economical.

The Pebble Bed Modular Reactor (PBMR) falls under this category. It is a high temperature graphite-moderated helium-cooled reactor [1]. The PBMR is to be constructed in South Africa but presently is in its design phase. This design is an improvement from the AVR reactor (Arbeitsgemeinschaft Versuchsreaktor) that was operated in Germany between 1967 and 1988.

The fuel design of the PBMR is spherical in shape, and is commonly known as a pebble. The reactor core contains approximately 452,000 of these pebbles, each of which
has a diameter of 6 cm. Each pebble has two regions: the fuel region is 5 cm in diameter, and the graphite shell has a thickness of 0.5 cm. The fuel region of the pebble contains about 15,000 small uranium oxide (UO₂) spherical particles (known as fuel kernels) enriched to about 9.6% (see Figure 1.1) [3]. Each fuel kernel is 0.9 mm in diameter and has four layers of coating. The first coating is the buffer of low-density graphite. It is followed by two layers of pyrolytic carbon which are separated by a layer of silicon carbide. These kernels are embedded in a graphite matrix to make up the 5 cm fuel region. Experiments have indicated that the use of coated particles embedded in a graphite matrix retain the fission products at fuel temperatures of up to 1600 °C. This is clearly one of the advantages of this design of the fuel.

Figure 1.1: The PBMR Pebble Fuel
The pebbles are packed in a reactor core with a packing fraction of about 0.61 to 0.64. The PBMR core is designed to have an annular core with an outer diameter of 3.7m, a fixed central graphite reflector with an outer diameter of 2m and a graphite side reflector which is 0.9m thick [3]. The core height is 11m. It is enclosed in a vertical steel pressure vessel which is 6 meters in diameter and 20 meters high. It is estimated that each pebble will be circulated through the reactor about 6 to 10 times, and will have a lifespan of about three years with an average residence time of 930 FPDs (Full Power Days). The average discharge burnup is 92,000 MWD/T (megawatt days per ton of uranium). Figure 1.2 illustrates the design of the PBMR reactor core [3].

1.2 Reactor Core Analyses

The importance of accurate nuclear cross sections cannot be overstated. Accurate nuclear cross sections are required for generating valid local fast and thermal reaction rate profiles that are the basis of safety analyses and nuclear material inventories. Equally as important, are the methods and the tools (computer codes) used in performing such analyses. For the PBMR, the given complexities of re-circulating graphite-laden fuel pebbles and high fuel discharge burnup levels make the problem more complicated and the choice of methods rather limited. There is hence the need to develop more accurate methods to analyze this reactor.
Figure 1.2: The Schematic of a PBMR Core
There are very few state-of-the-art analysis tools to model the pebble bed-type reactor, given the heterogeneity and the complexity of the design. Methods that are mostly in use today were developed more than twenty years ago. New developments and improvements in diffusion and transport methods have since surfaced, most of which have been for Light Water Reactors (LWR). Therefore there is a need to improve existing tools using more advanced methods. Accuracy and efficiency are the key drivers in improving these existing methods.

1.3 Current LWR Practice

The optimal balance between accuracy and efficiency in LWR analysis is achieved using a few-group nodal diffusion methodology. In this methodology the reactor core is divided into nodes which in a radial plane consist of a fuel assembly. Based on this nodal division of the core material compositions are defined for each composition, and few-group homogenized cross-sections are generated. The cross-section dependencies on exposure, history and instantaneous feedback parameters are functionalized in the form of cross section libraries. Usually these cross sections are generated in single assembly calculations in infinite geometry and the effect of the assembly environment into reactor core is either neglected or approximated through the criticality spectrum corrections or the more sophisticated approach of using “color sets”. For LWRs, the size of a fuel assembly is about 10 to 20 mean free paths, influenced by the fact that hydrogen is a moderator in this type of core. Thus, after a few mean free paths in the outlying zone of the color set, the spectrum in an assembly is the correct one,
regardless of the correctness of the boundary conditions on the outer edge of the color set. Hence it is an acceptable approximation in LWRs to ignore the remainder of the environment or its implied spectral effect.

In PBR core analysis the effect of the environment or surrounding region on pebble cross sections is very strong and cannot be neglected [4][5]. The fact that there is a continuous flow of pebbles in the core, a relatively large axial temperature gradient and neighboring fuel pebbles at different burnup levels, makes the spectral effects even more significant for core analyses. The reflectors in the PBR design (central, side, top and bottom reflectors) bring additional effects to the neutron spectrum for fuel pebbles closer to these regions. With graphite as a moderator, many more collisions are needed before the neutron is thermalized. This makes the neutron spectrum of PBRs significantly different (harder) as compared to that of hydrogen-moderated cores.

The diameter of the pebble is roughly one neutron mean free path. Thus after one pebble diameter from an interface between zones with different spectra, the effect of the neighboring spectrum still exists and cannot be ignored. In the current generation of HTR core simulation codes, the environmental effect is usually taken into account through spectrum (buckling or leakage) cross section feedback modeling for selected spectral zones. For the sake of efficiency of core calculations, a spectral zone consists of many pebbles. The corresponding local spectrum is therefore a function of the burnup mixture and the leakage spectrum. As a result, the proper selection of spectral zones is essential for PBR core analysis in order to model the environmental effect correctly.
1.4 Objectives of this Research

The objective of this PhD research is to improve the existing multigroup diffusion theory-based reactor core analysis of the Pebble Bed-type Reactors. The following are the two main research areas of investigations with unique PhD contributions:

- Development of a reference methodology for determining the reactor core spectral zones
- Development of a practical methodology for determining spectral zones using spectral indices

The main purpose of this research is to develop a methodology for automatically dividing the pebble bed-type of a reactor into spectral zones in order to perform more accurate diffusion theory reactor core calculations. The developed method will assist the reactor designer and analyst to systematically choose appropriate spectral zones for the reactor. A secondary research goal is to investigate the reactor physics characteristics of a spectral zone that establish the spectral zone boundary without need to always first have available a detailed transport solution.

Reactor physicists and nuclear engineers divide the core into regions (zones) and generate few-group homogenized (averaged) diffusion parameters over these regions. Then they perform the core calculations with average zone constants and the average flux spectrum. Although the zone averaged constants are obtained using sophisticated methods intended to ensure the equivalence of the heterogeneous and homogenized solutions, the discretization into large homogenous zones introduces some inaccuracies in the few-group cross sections. Additionally, the effect or influence of the neighboring
zones on the zone under consideration is not always optimally accounted for. The significance of this research is in the development of the methodology capable of providing a ‘recipe’ for dividing the core into appropriate zones which will yield more accurate results. The selection of these zones will be such that the core calculation results are within an acceptable tolerance as compared to a proper reference solution. This is achieved by choosing spectral zones through minimizing the error between the diffusion code solution and the reference transport solution. Furthermore, since the users may not always have a proper reference solution to a given reactor design, the method that was developed through this research also provide an alternative and more efficient approach to determining the spectral zones without the need for a reference solution.

When comparing the diffusion code output with the reference transport solution, it is important to ensure that for each zone selected, the following items are conserved:

- The power distribution
- The reaction rates in each zone
- The leakages into or out of each zone
- The effective multiplication factor

The physical state of the reactor also has an influence on the analyses: the fuel temperature and burnup (or fuel depletion) cannot be ignored in performing the analyses. The choice of analyses tools and the energy group structure also have direct influence on the results. These aspects are discussed in this dissertation.
1.5 Layout of the Dissertation

The literature review is presented in Chapter 2.

Chapter 3 details the cross section generation methodology. Other aspects of cross section generation and parameterization through the use of multi-dimensional cross section tables are presented. The work done for the PBMR 268MW [2] and PBMR 400MW [6] benchmarks in generating cross section tables is also outlined.

Chapter 4 presents MCNP as tool for generating the reference transport solution for all reactor models presented in this dissertation.

Chapter 5 addresses the selection of the appropriate energy group structure for this research work.

Chapter 6 focuses on the theory of spectral zone selection methodology. The Equivalence Theory and how it is applied to this research is discussed in detail. The optimization algorithm designed to identify spectral zones is presented in this chapter.

The methodology for determining the spectral zones using diffusion-only spectral indices is discussed in Chapter 7.

Chapter 8 focuses on the selection of spectral zones in the axial dimension.

Chapter 9 addresses the selection of spectral zones in the reflectors.

Chapter 10 presents practical application of the developed methodology to actual reactor core problems.

The conclusions and recommendations for future work are summarized in Chapter 11.
Chapter 2

Literature Review

The High Temperature Gas-cooled Reactor (HTGR) exhibits some unique reactor physics features that distinguish it from Light Water Reactors (LWR). Some of the important features of the HTGR and key differences from the Light Water Reactors are discussed in this chapter. Some important reactor physics concepts are also discussed.

2.1 High Temperature Gas-cooled Reactors

Several high temperature gas cooled reactors have been operated in the past. The DRAGON reactor was a 20MW reactor that reached its nominal power in Winfrith, England in 1966 [7]. The Peach Bottom Reactor Unit 1 which was constructed in Pennsylvania USA, reached its full power operation in 1967. It was a 200MW reactor designed by General Atomic of San Diego. It was shutdown in October 1974. The AVR pebble bed reactor was a 40MW reactor which was operated from 1967 to 1988 in Jülich Research Center, West Germany. The Fort Saint Vrain in Colorado USA reached initial criticality in 1974. It was operated commercially from 1976 to 1989.

One of the unique features of HTGRs is the use of graphite as a moderator, which has a very low absorption cross section. Helium is used as a coolant, selected because of its properties. It is chemically inert, does not undergo any phase change, has good heat-
exchange properties and it is not activated by neutrons [7]. Additionally it is available in sufficient quantities.

The fuel design is also unique. Small uranium oxide (UO$_2$) spherical particles about 200 to 800µm in diameter are coated with layers of graphite and silicon carbide. The first inner layer is a low density buffer layer, followed by high density pyrolytic carbon layer. The silicon carbide layer is the third layer, followed by the fourth (and last) high density pyrolytic carbon layer. It is these layers that retain the fission products at fuel temperatures of up to 1600 °C. The coated particles are put together in a matrix of graphite powder.

With this design of the fuel, graphite as the moderator and helium as a coolant, high gas temperatures in the region of 900°C are attained. This is a very high coolant temperature compared to the coolant outlet temperatures in LWRs of about 300°C. This results in high power conversion efficiency in HTGRs. It has also been shown that the fuel because of it design, can reach high burnup levels.

In the recent past the interest of HTGR technology has significantly increased. There are various research initiatives carried out globally [8][9]; with some collaboration of research efforts to validate safety-related physics calculations and to improve existing methods. The need to develop an advanced nuclear power reactor that is safe, reliable, economical, sustainable, and that has proliferation-resistant qualities, make the HTGR a very attractive reactor for the new generation of nuclear reactors.
2.2 Review of Transport Theory

One of the most important activities of a reactor designer and physicist is to be able to accurately determine the behavior and balance of neutrons in the reactor. The behavior of neutrons can be described using the neutron transport equation which is given by the linear form of the Boltzmann equation, assuming that the neutrons do not interact with each other. This is given by Eq. 2.1 [17].

\[
\frac{\partial n}{\partial t} + \nu \hat{\Omega} \cdot \nabla n(r, E, \hat{\Omega}, t) + \nu \Sigma, n(r, E, \hat{\Omega}, t) = \int_{4\pi} d\hat{\Omega} \int_{0}^{\infty} dE' \nu \Sigma, (E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) n(r, E', \hat{\Omega}', t) + s(r, E, \hat{\Omega}, t)
\]  

(2.1)

Where \( \frac{\partial n}{\partial t} \) is the time rate of change of the neutron density. The different terms of the transport equation are explained as follows;

**Leakage term**

\( \nu \hat{\Omega} \cdot \nabla n(r, E, \hat{\Omega}, t) \) is the term defining the neutrons leaking out of the system.

**Collision term**

\( \nu \Sigma, n(r, E, \hat{\Omega}, t) \) is the rate at which neutrons suffer collisions at point \( r \). This is based on all types of collisions: elastic and inelastic scattering, and all forms of absorptions.

**Scattering term**
\[ \int_{4\pi} d\hat{\Omega} \int_0^\infty dE' v' \Sigma_s(E' \rightarrow E, \hat{\Omega}' \rightarrow \hat{\Omega}) n(r, E', \hat{\Omega}', t) \]

represents a gain of neutrons due to scattering into \( dE \) about \( E \), \( d\hat{\Omega} \) about \( \hat{\Omega} \) from other energies \( E' \) and directions \( \hat{\Omega}' \).

**Source term**

\[ s(r, E, \hat{\Omega}, t) \] is the source term which represents the source of neutrons.

Solving the neutron transport equation is complicated by the dependence of the parameters on space, energy, angle and time. The solution can be achieved by first discretizing each of the variables in the equation and converting the equation into a system of algebraic equations. For example the energy dependence is discretized into a high number of energy groups due to the high dependence of cross sections on energy. There are various methods available in literature [10][17][18] that can be used to accomplish the discretization of the neutron transport equation. These are not discussed in this dissertation.

### 2.3 Review of Multigroup Diffusion Theory

Neutron transport theory tools may be complex and very expensive to execute for routine design and safety calculations; hence an alternative to solving the neutron transport theory was developed. Neutron diffusion theory is such an alternative to solving the neutron transport equation. This approximation is valid based on certain assumptions. One assumption is that the angular distribution of neutron velocity vectors is isotropic, or
nearly isotropic [17]. Diffusion theory is only valid in regions that are some distance away from sources or boundaries. This theory allows for calculations of various phenomena taking place in the reactor without the details and the effort of solving the neutron transport equation.

The underlying principle of the diffusion theory is to be able to determine the balance of neutrons in the reactor as accurately as possible [20]. This balance is determined from the production, absorption and leakage of neutrons and translates in practice into solving the diffusion equation presented in Eq. 2.2:

\[
\frac{1}{\nu} \frac{\partial \phi}{\partial t} = D \nabla^2 \phi(r, E, t) - \Sigma_a \phi(r, E, t) + s(r, E, t)
\]  

(2.2)

where:

\[ \frac{1}{\nu} \frac{\partial \phi}{\partial t} \text{ is the rate of change of the neutron flux} \]

\[ D \nabla^2 \phi \text{ is the leakage rate of neutron out of the system} \]

\[ \Sigma_a \phi \text{ is the absorption reaction rate} \]

\[ s \text{ is the source of neutrons in the system} \]

\[ (r, E, t) \text{ indicates the dependence on space, energy and time} \]

Generally this equation is solved with the use of computer codes. The most accurate way of solving the diffusion equation is to solve for the balance of neutrons in many energy groups [41][42]. In this manner the slowing down of fast neutrons in thermal reactors is treated in a more realistic approach as opposed to the two-group theory. Eq. 2.3 is the multi-group form of the diffusion equation [18].
\[
\frac{1}{v_g} \frac{\partial \phi_g}{\partial t} = D_g \nabla^2 \phi_g (r) - \Sigma_{sg} \phi_g (r) - \Sigma_{ag} \phi_g (r) + \sum_{g'}^{G} \Sigma_{g' \rightarrow g} \phi_{g'} (r) + \chi_g \sum_{g'=1}^{G} v_{g'} \Sigma_{sg'} \phi_{g'} (r)
\]

(2.3)

where:

\( \frac{1}{v_g} \frac{\partial \phi_g}{\partial t} \) is the rate of change of the neutron flux in group \( g \)

\( D_g \nabla^2 \phi_g \) is the leakage rate of neutron out of the system in group \( g \)

\( \Sigma_{ag} \phi_g \) is the absorption reaction rate in group \( g \)

\( \Sigma_{sg} \phi_g \) is the scattering reaction rate in group \( g \)

\( \Sigma_{g' \rightarrow g} \phi_{g'} \) is the upscattering reaction rate from group \( g' \) to group \( g \)

\( \chi_g \) is the probability that a fission neutron will be born with energy in group \( g \)

\( \Sigma_{sg'} \phi_{g'} \) is the fission reaction rate in group \( g' \)

\( v_{g'} \) is the average number of neutrons released in a fission reaction induced by neutron in group \( g' \)

There will be as many diffusion equations as there are energy groups in a given problem. Also each region of the reactor is characterized by its own set of equations. For instance if there are two reactor regions; the reflector and core regions, the diffusion equation will be solved for both these regions for a given number of energy groups.
Solving the diffusion equation for many groups by hand is extremely difficult (if not impossible); the calculations are performed on computers. For some reactors, such as Light Water Reactors, it is generally acceptable to solve the equation in two groups only; assuming the neutrons are divided into fast and thermal energy groups only.

Graphite has a low average logarithmic energy decrement per collision compared to hydrogen as a moderator in Light Water Reactors [21]. It follows that more collisions are necessary to slow the neutrons to thermal energies. Therefore multigroup diffusion equations are required for graphite-moderated reactors. This topic is further discussed in Chapter 5. Four groups and higher are generally used for HTGRs, with the accuracy of the analysis improving with the higher number of energy groups.

2.4 Limitations of Diffusion theory

The diffusion equation discussed in the previous section, is based on the following four assumptions [17]:

- The angular flux can be adequately represented by a linearly anisotropic angular dependence
- One speed neutron density
- Isotropic scattering
- The neutron current density changes slowly compared to the mean collision time

The first assumption is the most important and is violated under certain conditions. Thus the diffusion equation will not be valid:
- Near the boundaries or where material densities change significantly
- Near the sources
- In a strong absorbing medium

Based on the above, it would be expected that the discrepancy between a transport solution and a diffusion solution would exist at the core-reflector interfaces.

In practice, for LWRs a transport theory correction factor has been developed and applied at the core-reflector interfaces to correct the flux calculations.

### 2.5 Energy Group Structures

As mentioned earlier in this chapter, multigroup equations are required to solve the diffusion equation for the graphite-moderated reactors. This is based on the fact that the fast neutrons suffer several interactions with the moderator before they are thermalized. Secondly, in the thermal groups where upscattering cannot be ignored, the group boundaries are more important in the regions of low-lying plutonium resonance.

A variety of group structures exists for the analysis of high temperature reactors. Several group structures have been identified in [7]. A group structure with a higher number of groups would produce the $k_{eff}$ and the power distribution with better accuracy. However such group structures would be computationally expensive. Therefore a balance is struck between accuracy and computational costs.

A 13-group structure has been used with MICROX-2 [15]. Other group structures between 4 groups and 9 groups are identified in [7]. However there is no set of group structures that are recommended or regarded as the best group structures for HTGRs.
A sensitivity study was carried out at Penn State University to investigate the best group structures for the PBRs [19]. Several group structures were identified in this report together with the recommended group structures. The issue of group structures is investigated further in Chapter 5.
Chapter 3

Cross Section Generation Methodology

3.1 Overview

Cross sections are an important parameter in nuclear reactor modeling. They are an integral part of core design, fuel management, fuel optimization and all nuclear reactor core analyses. Incorrect generation and processing of cross sections leads to inaccurate core analyses. Therefore the importance of accurate cross section data cannot be overstated.

The basis of all nuclear cross sections is the nuclear data libraries. Various sets of data have been put together into a convenient Evaluated Nuclear Data File (ENDF). The file contains the continuous energy-dependent evaluated cross section data of many materials. Each material file contains a series of data such as neutron cross sections, resonance data, energy distributions, thermal scattering law data, etc. A cross section processing code is required to repackage the data into user-specific data form relevant to a problem under investigation.

There are various steps necessary for the generation and processing of cross sections to obtain the specific data that one can apply to a given core analysis problem. The process is influenced by the choice of processing codes.

The fine group cross section library is generated using the ENDF data where cross sections are averaged over this fine structure using appropriate weight functions [13][17].
This fine group data is used in a unit cell to obtain a spatial flux distribution and subsequently homogenized over the unit cell. Using the fine group homogenized flux spectrum, a weighting technique is applied to average or collapse the cross sections into broad group cross section library where the broad group cross-sections are further homogenized over a larger region such as an assembly or a spectral zone. This broad group library is then ready for use in core calculations using static or kinetics codes.

3.2 Cross Sections Feedback Model

There are various tools and methods that are available for generating nuclear cross sections. The major improvements in methodologies for the generation of cross sections have been mainly focused on the Pressurized Water Reactor (PWR) and Boiling Water Reactor (BWR). Cross sections are sensitive to changes in temperature and material number densities which affect the spectrum. Such changes in the reactor conditions require that cross sections be updated to accurately reflect the conditions in the core. One of the methods suggested by Watson and Ivanov [12] is the Adaptive High Order Table Look-up Method (AHTLM). The accuracy of cross section modeling is improved by interpolating into multi-dimensional cross section tables which include all the bounding cases of the core.

The parameterization model of cross-section dependencies in a PBMR usually accounts for the feedback effects of temperature, spectrum and Xenon. In such a feedback model the cross-sections are calculated for each spectral zone and for each coarse energy group.
The basic unit of material composition is a batch (see Figure 3.1). In each layer a number of batches with different irradiation ages can reside. These are mixed and put together to form a layer. These layers present partial volumes of the reactor core, which provide the distribution of materials (or cross sections) for the flux calculation. All the batches within a layer are exposed to the same local flux. A number of batches can be

Figure 3.1: Schematic of PBMR Spectral Zones
placed together to form a spectral zone. Spectral calculations are based on the averaged atom densities of all the batches within this zone and therefore provide the broad group cross sections for the respective batches.

The major PBMR reactivity feedback parameters are fuel temperature and moderator (graphite) temperature, the spectrum and Xenon concentration. The spatial variation of these parameters requires a proper modeling of local cross-section dependencies on these feedback parameters for a multi-dimensional PBMR core analysis. In the AHTLM approach for PBMR application the entire ranges of changes of the major feedback parameters are covered using multi-dimensional table interpolation thus avoiding simplified polynomial fitting with possibilities for extrapolation. The cross section representation methodology developed at PSU not only uses the cross section at average conditions but also uses the cross term cross sections. Cross-term cross sections are cross sections calculated by varying two or more parameters at the same time. This method takes into account the non-linear feedback parameter phenomena that may be critical for accurate prediction of the cross section behavior.

Multidimensional cross section tables were developed for the PBMR 268MW benchmark [2] with dependence on the following parameters:

- Fuel temperature
- Moderator temperature
- Fast buckling
- Thermal buckling
- Xenon concentration
The cross-section library is dependent on fuel temperature, moderator temperature, the xenon concentration, and geometrical buckling representing the environment spectrum and leakage feedback effects. The difference in fuel and moderator temperatures is particularly important during transients where the two temperatures can vary considerably. Fast and thermal bucklings account for the leakage (in or out of the system). The Xenon state parameter accounts for spectrum changes due to the large thermal absorption cross section of Xenon.

The script for the table lookup was developed using visual basic. The cross sections were developed using a system of three codes: NJOY [13], MICROR [14] and MICROX-2 [15]. All diffusion cross sections generated for the entire work in this dissertation were generated with the same code system.

3.3 A System of Cross Section Generation Codes

NJOY [13], MICROR [14] and MICROX-2 [15] are the three codes that were used in the cross section generation of the PBMR model that were investigated. NJOY is a nuclear data processing code that processes the evaluated nuclear data and produces the point-wise (PENDF) and multi-group (GENDF) cross sections. MICROR is a reformatting module. It reformats the PENDF and GENDF cross sections from NJOY and produces three output files: FDTAPE, GARTAPE and GGTAPE. MICROX-2 is a one-dimensional two-region lattice cell code. It uses the three output files from MICROR to produce broad group cross sections for use in diffusion and transport codes. This scheme is presented in Figure 3.2.
The NJOY code is a nuclear data processing system which produces point-wise and group-wise cross sections from the ENDF. The code converts the evaluated nuclear data into libraries useful for application calculations in nuclear engineering problems. The data is converted from the ENDF format to the Point-wise Evaluated Nuclear Data File (PENDF) format and Group-wise Evaluated Nuclear Data File (GENDF) format.

The ENDF data was obtained from Los Alamos National Laboratory. There are a number of versions of ENDF available. For this project, ENDF-B/VI was used with the NJOY version 99.161.

Figure 3.2: A System of Cross Section Generation Codes

3.3.1 NJOY

The NJOY code is a nuclear data processing system which produces point-wise and group-wise cross sections from the ENDF. The code converts the evaluated nuclear data into libraries useful for application calculations in nuclear engineering problems. The data is converted from the ENDF format to the Point-wise Evaluated Nuclear Data File (PENDF) format and Group-wise Evaluated Nuclear Data File (GENDF) format.

The ENDF data was obtained from Los Alamos National Laboratory. There are a number of versions of ENDF available. For this project, ENDF-B/VI was used with the NJOY version 99.161.
The NJOY code consists of a number of modules. Each module operates as a separate computer program, processing a well-defined task. This feature makes it possible to choose only the modules that are relevant to a specific problem. The modules are linked by input and output files. The following modules were used in processing the ENDF-B/VI data for the PBMR cross section generation project:

- RECONR
- BROADR
- HEATR
- UNRESR
- THERMR
- GROUPR
- MODER

The RECONR module reconstructs resonance cross sections from ENDF resonance parameters. It also reconstructs the cross sections from nonlinear interpolation schemes. It reads the ENDF-format tape and produces a common energy grid for all neutron reactions such that all cross sections can be obtained (within a specified tolerance) by interpolation. The output is written onto a PENDF tape.

The BROADR module reads the PENDF tape from RECONR, and Doppler-broadens the thin point-wise resonance cross sections for different temperatures. This module uses the kernel broadening method, also known as the SIGMA1 method, but modified for better behavior at high temperatures and low energies. The output is written onto a new PENDF tape.
The UNRESR module computes the effective self-shielded point-wise cross sections for resonance reactions in the unresolved resonance region. The unresolved range begins at the energy where it is difficult to measure an individual resonance. It extends to the energy where the effects of fluctuations in the resonance cross sections become unimportant. The UNRESR module averages the values of resonance widths and spacing distances together with distribution functions for the widths and spacing distances. This representation is converted into effective cross sections. The module uses the ENDF tape and the PENDF tape from BROADR as input. The computed effective cross sections are written onto a new PENDF tape.

The HEATR module generates point-wise heat production cross sections for specified reactions. Neutron heating arises from the kinetic energy of the charged products of a neutron-induced reaction. It is proportional to the local neutron flux. The module uses the ENDF tape and the PENDF tape from UNRESR as input. The output is written onto a new PENDF tape.

The THERMR module generates point-wise neutron scattering cross sections in the thermal energy range. It produces inelastic cross sections and energy-to-energy matrices for free atoms or bound scatters. THERMR module uses the ENDF tape and the PENDF tape from UNRESR as input. The output is written onto a new PENDF tape.

The GROUPR module generates self-shielded multi-group cross sections and group-to-group neutron scattering matrices. This module uses the ENDF tape and the PENDF tape from THERMR as input. The output is written onto a GENDF tape.
The MODER module converts the data from formatted mode (e.g. ASCII) to blocked-binary mode, and vice versa (from blocked-binary to formatted mode). A formatted file has a positive unit number, while a binary file has a negative unit number.

There are other NJOY modules that were not necessary for the purpose of this project, and were thus not used and hence not included in this discussion. The ACER module was necessary for the generation of MCNP continuous energy cross sections. The discussion on this module is addressed in Section 3.5 (MCNP cross section generation).

### 3.3.2 MICROR

MICROR is a reformatting module that uses the two output files from NJOY; PENDF and GENDF. It produces three output files: FDTAPE, GARTAPE and GGTAPE. These three files serve as input files to MICROX-2. FDTAPE contains the fine group dilution- and temperature-dependant cross sections in the fast energy range. GARTAPE contains point-wise Doppler broadened resonance cross sections in the resolved resonance range. GGTAPE consists of infinite dilution cross sections in the thermal energy range. GGTAPE also contains data in the fast range; however this is not used by MICROX-2.

FDTAPE contains cross section in the energy range from 2.38 eV to 1.49E+07 eV. These cross sections are prepared from the GENDF file (output file from GROUPR module in NJOY). The file includes all cross sections for the specified reactions in GROUPR; elastic scattering, inelastic scattering, radiative capture, fission and absorption reactions, and all the other (n, xn) reactions.
The resonance cross sections are calculated from the PENDF data prepared by RECONR and BROADR modules in NJOY and stored in the GARTAPE. The required accuracy of the reconstruction and resonance integrals is specified in these two modules. The energy point distribution is obtained using the method of cross section linearization. The two options available are the equidistant lethargy and velocity energy point distribution. Both of these options lead to a reasonable number of energy points in the resonance range. In strict terms, the velocity energy point distribution option is more appropriate for fast reactor systems while the equidistant lethargy option is more relevant for thermalized systems.

The thermal energy range in the GARTAPE is from 0 eV to 2.38 eV. The thermal neutron cross sections are recorded in the thermal section of the GGTAPE. These cross sections are prepared from the THERMR and GROUPR output files. Both elastic and inelastic scattering matrix specified in GROUPR are considered.

### 3.3.3 MICROX-2

MICROX-2 is an integral transport theory code [15]. It solves the B1 neutron balance equations in a one-dimensional two-region unit cell and obtains the neutron weighting spectrum. The two regions are coupled by collision probabilities based on a spatially flat neutron emission (not flat neutron flux). Dancoff factors and buckling terms correct the one-dimensional cell calculations for multi-dimensional lattice effects. MICROX-2 prepares the broad group neutron cross sections for use in diffusion and transport codes. It can process up to 11 mixtures and a maximum of 13 fission spectra for each spatial region. It has three geometry options: spherical, cylindrical and planar (slab).
For the PBR, a spherical representation of the pebble and the surrounding gap is illustrated in Figure 3.3. In MICROX-2 the inner region of the fuel unit cell contains fuel particles (also called kernels or grains). The code has the capability of treating two types of grains in this region. The two grain types, grain coatings and the matrix material can be modeled explicitly in this region. The outer region consists of the shell/moderator/coolant. For the spherical geometry as in the case of the PBMR pebble fuel, the two regions of the pebble cell (see Figure 3.4) are distinguished as follows:

- Region 1 consists of the inner fuel region. This is the 5cm diameter region that contains the fuel kernels in the graphite matrix. Only one type of grain is specified in the PBMR model since the fuel has only one type of grain.
- The graphite shell and the coolant are homogenized into one region to form Region 2. The volume of the coolant depends on the specified packing fraction of the pebbles.

The 193 General Atomics group structure [14] is used as a fine group structure, with $1.49 \times 10^7$ eV as the upper boundary of the first group. The complete 193 group structure is included in Appendix A. The fast/thermal energy cutoff is fixed at 2.38 eV. MICROX-2 allows a fission spectra combination of up to thirteen fissionable isotopes. The user-specified fission spectrum weights are used to normalize the space and energy integral of the spectra. Isotropy is assumed for the fission contributions to the fine group sources.
Figure 3.3: Spherical Fuel Cell

Figure 3.4: PBMR Fuel Model in MICROX-2
The Benoist Spatial Weighting is a method used for the spatial weighting of the transport mean free paths of different media in a multi-region cell. The weighted transport mean free paths are used to correct the cell leakage. This method is used in preparation of the direction-averaged diffusion coefficients, and applies even when one of the media is void. The cell-averaged isotropic diffusion coefficient is averaged over all directions in a regular infinite lattice.

Bucklings are used to specify the leakage into or out of a region. One of the good features of the code is that the group bucklings can be supplied for each of the fast and thermal broad groups. This has proved to be very useful for this research since it allowed for proper optimization of the group-dependent bucklings.

3.4 Buckling and Leakage Feedback

Different codes apply different methods or approaches to account for the leakage feedback. In VSOP for instance [16], the leakage feedback is incorporated differently in GAM (fast spectrum code) and in THERMOS (spectrum cell calculations in the thermal energy range). In the epithermal energy range, the leakage terms are transferred into bucklings. These terms are then passed on to the GAM code for the P1 approximation of the transport equation. A single value of the average buckling was traditionally used, as opposed to entering bucklings into corresponding fine groups adapted more recently.

When generating PBMR cross-section libraries it is very important to model the spectrum dependence. The utilized assumption in the PWR cross-section generation and modeling methodology that the neutron spectrum within a fuel assembly is dominated by
the material composition and burn-up of the assembly is not valid for the small PBMR fuel spheres and the graphite moderation environment [4]. The spectrum within a fuel sphere is mostly determined by the material compositions and burn-up of surrounding spheres. The first consequence of this fact is that the cross-sections have to be generated using a reactor model (color-set calculations) rather than single assembly calculations (as it is usually done in the PWR case). The second consequence is that the cross-sections should be represented as a function of some spectral parameter as for example the leakage term or buckling. Leakage of neutrons from/to the adjacent spectral zones is included by buckling terms, which are generated from the diffusion calculation over the whole reactor.

From the 3-D diffusion run, leakage terms are calculated for each spectral zone and for each coarse energy group. Four energy groups are normally used. The leakage of the cell is equal to the leakage from the spectral zone divided by the zone volume. From the core diffusion calculation the leakage term for the spectrum feedback is obtained. The core thermal-hydraulic model provides the corresponding temperatures of the fuel and moderator averaged over the volumes of the reactor spectral zones, and thus ready for further neutronics evaluation. The VSOP layer macroscopic cross sections are determined from the microscopic cross sections obtained from GAM and THERMOS (spectrum calculation) and the number densities (and volume fraction) of each batch of fuel in that layer.

The approach implemented in MICROX-2 is slightly different. The Benoist Spatial Weighting is a method used for the spatial weighting of the transport mean free paths of different media in a multi-region cell [15]. The weighted transport mean free
paths are used to correct the cell leakage. This method is used in preparation of the direction-averaged diffusion coefficients, and applies even when one of the media is void. The cell-averaged isotropic diffusion coefficient which is averaged over all directions in a regular infinite lattice is determined by Eq. 3.1:

\[
3D_c = \frac{\sum_i \sum_j V_i \phi_i \lambda_j P_{ij}}{\sum_i V_i \phi_i}
\]

(3.1)

where: \( D_c \) is the cell- and direction-averaged diffusion coefficient

\( V_i \) is the volume of medium \( i \),

\( \phi_i \) is the average flux in medium \( i \),

\( \lambda_j \) is the transport mean free path in medium \( j \), and

\( P_{ij} \) is the source transfer probability from region \( i \) to \( j \).

The spatial flux weighting of \( P_0 \) Legendre moment cross sections are calculated using Eq. 3.2. The spatial weighting of \( P_l \) and higher Legendre moments \((l \geq 1)\) cross sections are determined using Eq. 3.3.

\[
\Sigma_{c,0} = \frac{\sum_i V_i \phi_i \Sigma_i}{\sum_i V_i \phi_i}
\]

(3.2)

\[
\Sigma_{c,l} = \frac{\sum_i V_i \phi_i \Sigma_i}{\phi_c}
\]

(3.3)
where: $\dot{V}_i$ is region $i$ volume fraction in the unit cell, and

$\omega_i$ is the spatial weighting factor used for averaging the transport cross sections.

The method for the determination of $\omega_i$ depends on the Benoist spatial weighting option that the user selects. The user has a total of three options.

Bucklings are used to specify the leakage into or out of a region and are defined by Eq. 3.4 [15]

$$L = DB^2 \phi V$$  \hspace{1cm} (3.4)

where: $L$ is the neutron leakage into or out of a region (n.s$^{-1}$),

$D$ is the diffusion coefficient (cm),

$B^2$ is the buckling (cm$^{-2}$),

$\phi$ is the average neutron flux (n.cm$^{-2}$.s$^{-1}$)

$V$ is the volume of the region (cm$^3$)

Leakage of neutrons across the adjacent spectral zones is included by buckling terms, which are generated from the diffusion calculation over the whole reactor, and are subsequently used in the B-1 or B-3 approximations to the 1-D transport equation solved for MICROX-2 to account for the leakage out of the cell. The code checks that the leakage into the region is less than the removal. This is done by ensuring that the value of the negative buckling is less than the macroscopic removal cross section. If the leakage into the region exceeds the removal, the code will either stop or reduce the value of the negative buckling to half the value of the removal cross section. These two options are selected by the user.
There is another option available to perform the just critical buckling calculation. When this option is selected, the input bucklings are multiplied by a constant factor so that the computed effective multiplication factor $k_{\text{eff}}$ is one. This implies that the energy dependence of the input bucklings is not changed during the buckling search. The recommended initial value for the bucklings is $1.0 \times 10^{-10} \text{ cm}^{-2}$.

Leakage calculations are normally the biggest source of error in many analyses tools. It is therefore necessary that the approach is further explored to ensure that the bucklings as used in MICROX-2, are the most efficient and accurate way to represent the leakage.

### 3.5 MCNP Continuous Energy Cross Sections

The MCNP code [24] has a built-in cross sections library that contains several library files. The one limitation of this library is that the temperatures at which these libraries were generated, is very limited. In fact most of the library files were generated at room temperature. It was therefore necessary to generate a specific library that would cover all temperature ranges and all materials needed for this research.

#### 3.5.1 Generation of MCNP Cross Sections with NJOY

MCNP continuous energy cross sections are generated using the NJOY code [13]. The same NJOY version (99.161) is used as with the MICROX-2 cross sections. All the NJOY modules discussed in Section 3.3 are also included in the procedure, with the
exception of GROUPR. Two new modules are added; the PURR module and the ACER module.

BROADR and RECONR modules are necessary to ensure that all cross sections are presented on a union energy grid that is suitable for linear interpolation. The UNRESR module generates the unresolved self-shielding cross sections which are suitable for use after processing with GROUPR. However since GROUPR is not needed for the generation of continuous energy cross sections, the unresolved self-shielded data is not very accurate and therefore not very useful for MCNP applications. Therefore an additional module, PURR is necessary for producing the probability tables. MCNP uses the “Probability Table” method for treating the unresolved resonance self shielding cross sections.

The ACER module processes cross sections into the ACE format [13] [24] that are readable and readily useable by MCNP. The ACER is executed for each material/isotope of interest, one material at a time. The entire process is summarized in Figure 3.5.

The type of output file generated by ACER depends on the user-specified output format; binary or ascii file. All the output files are then put together into one library file. The MCNP directory file xsdir must be updated with the new library file name with its contents (list of materials).
Figure 3.5: Continuous Energy Cross Section Generation Process
### 3.5.2 Verification of the New Library

With the procedure outlined above for generating continuous energy cross sections for MCNP, it was necessary to validate the method and verify that the generated cross sections are accurate. For this, a simplified PBMR 268MW case 1 [2] was analyzed with the existing (built-in) library cross sections at 293K; this was considered to be a reference solution. The simplified model was based on a two-region reactor: the reactor core (fuel region) and the reflector. The same case was executed with the cross sections generated based on the above-described procedure. The effective multiplication factor ($k_{\text{eff}}$) and the total flux are compared in Table 3.1 and Figure 3.6 respectively.

| Table 3.1: $k_{\text{eff}}$ Comparison for Built-in and New Cross Sections at 293K |
|---------------------------------|---------------------------------|
| Built-in Cross Sections | New Cross Sections |
| $k_{\text{eff}}$ | 1.31243 ±0.00072 | 1.31240 ±0.00068 |
| % Difference | - | 0.0023% (3pcm) |

Table 3.1 and Figure 3.6 show a very good agreement of the two cases: one generated with the original MCNP cross sections, and the other with the new cross section library generated with NJOY99.161 based on the procedure described in the previous section. The results of the test show a very good agreement of the $k_{\text{eff}}$ and the flux. Also the power profiles were compared, and showed a very good agreement.
These results confirmed that the new cross sections were adequately and correctly generated. Cross sections of all materials at temperatures up to 1200K were generated using the same procedure.

![Graph of Total Flux for the Simplified 268MW Core](image)

**Figure 3.6**: Comparison of the Total Flux: Built-in and New Cross Sections at 293K

### 3.6 Conclusions

It has been demonstrated that proper tools for generating cross sections are needed to generate accurate cross sections. This emphasizes the need for a proper cross section generation methodology. Cross sections generated with the tools identified in this chapter have proved to be adequate for this research.
Chapter 4
Reference Calculations with MCNP

4.1 Monte Carlo N-Particle Code

The Monte Carlo N-Particle MCNP code is a continuous energy time dependent transport code [24]. Monte Carlo methods have a stochastic nature and are different from the deterministic transport methods. In the deterministic methods, the transport equation is solved by discretizing the problem in the phase space. The neutron balance is then solved for an average particle behavior in the defined discretized units. In Monte Carlo methods individual trajectories are simulated and aspects of their average behavior are recorded as tallies. There is no need to solve the transport equation; individual particles are tracked from their birth through probabilistic events to their death. Their behavior is tracked using the probability density functions based on randomly sampled distributions. The probability distributions are statistically sampled to describe the total phenomena. Averaging in the space, energy and time dimensions is not necessary since the Monte Carlo method does not use the phase space units.

The statistical sampling is based on the selection of random numbers. A high number of histories that track the events of each particle is needed to obtain good statistical average quantities. Based on the requested quantities of interest, the output is tallied with the statistical precision (or statistical error) of the results.
The Monte Carlo methods are very popular in nuclear reactor calculations because of the statistical nature of the method. The solution derived from this method is exact and no approximations are performed. This is because the results are based on the history of each particle. This makes the Monte Carlo-based code MCNP an ideal method and hence a computational tool of choice to develop an exact reference solution.

4.2 The Basis for a Reference Solution

The purpose of this research, as it has been described in Chapter 1 is to develop a methodology for determining optimum spectral zones using diffusion theory. The basis on which the methodology is developed is that the established spectral zones would yield a solution that is as close as possible to the reference solution. These spectral zones would form a basis for optimum reactor physics conditions for the diffusion code NEM [23] to yield a more accurate diffusion solution.

The basis of the Monte Carlo methods as described above makes the MCNP code a very attractive code for developing a reference solution. With the MCNP code, it is possible to specify the required quantities such as the flux and reaction rates in the tally specifications. This would then make it possible to compare these quantities with those based on the diffusion code. The solutions are not expected to be exact since diffusion theory is based on certain approximations and has some known limitations. With the cross sections developed as described in Chapter 3, a full reactor model is constructed and analyzed to give a detailed transport reference solution for this research.
4.3 PBMR400 Core Design

The development of the methodology for determining spectral zones PBRs is based on the actual PBMR design. The PBMR 400MW is the core design that was selected for this purpose. The PBMR400 benchmark [3] is a coupled neutronics/thermal hydraulics transient benchmark based on the PBMR 400MW design. The benchmark was initiated to test the tools and methods available to analyze a High Temperature Gas-cooled Reactor (HTGR), of which the PBMR is an example. The benchmark defines both steady state and transient cases. The detail included in the definition made this a design of choice to develop the methodology for determining spectral zones for PBRs.

Design Specifications of PBMR400

The PBMR 400MW core as defined in the benchmark [3] has an annular core with an outer diameter of 3.7m, a fixed central graphite reflector with an outer diameter of 2m and a graphite side reflector which is 0.9m thick. The core height is 11m.

The Reactivity Control System is situated in the side reflector. It consists of 24 partial length control rod positions with 12 upper control rods, and 12 lower shutdown rods. All 24 rods operate together during normal operation conditions. The Reserve Shutdown System is situated in the central reflector. It consists of 8 Small Absorber Spheres 1cm in diameter. The spheres contain $B_4C$.

The core is loaded with approximately 452,000 fuel pebbles with a packing fraction of 61%. The uranium loading is 9g per fuel sphere enriched to 9.6 wt%. The
continuous on-line multi-pass refueling scheme allows the fuel to be re-circulated at an average of 6 times. Fuel is discharged when burnup levels exceed 90,000 MWd/tU.

The benchmark design has been simplified in some ways to minimize potential source of errors and approximations. The upper surface of the pebble bed has been flattened, and the de-fueling channel at the bottom of the core was eliminated.

Some of the important design specifications based on the benchmark specification are included in Table 4.1.

<table>
<thead>
<tr>
<th>#</th>
<th>Description</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.</td>
<td>Equivalent core outer radius</td>
<td>m</td>
<td>1.85</td>
</tr>
<tr>
<td>2.</td>
<td>Cylindrical height of the core (Flattened core surface at the top and flat bottom reflector).</td>
<td>m</td>
<td>11.0</td>
</tr>
<tr>
<td>3.</td>
<td>Total core volume</td>
<td>m³</td>
<td>83.7155</td>
</tr>
<tr>
<td>4.</td>
<td>Fixed central column graphite reflector radius</td>
<td>m</td>
<td>1.0</td>
</tr>
<tr>
<td>5.</td>
<td>Effective annular thickness of the side reflector (graphite).</td>
<td>m</td>
<td>0.9</td>
</tr>
<tr>
<td>6.</td>
<td>Inner radius of the core barrel</td>
<td>m</td>
<td>2.88</td>
</tr>
<tr>
<td>7.</td>
<td>The wall thickness of the core barrel.</td>
<td>m</td>
<td>0.05</td>
</tr>
</tbody>
</table>
| 8. | Radii of five material meshes in core (5 radial material meshes in core, equal width) | m    | 1.17  
|    |                                                                             |      | 1.34      |
|    |                                                                             |      | 1.51      |
|    |                                                                             |      | 1.68      |
|    |                                                                             |      | 1.85      |
| 9. | Thickness of core radial meshes (all equal)                                 | m    | 0.17      |
| 10.| Axial material mesh: 11.0 m / 22 meshes (in core)                           | m    | 0.5       |
| 11.| Total height of top reflector                                               | m    | 1.5       |
| 12.| Total height of bottom reflector (Distance from top of bottom plate to bottom of core). | m    | 4.0       |

The material layout of the reactor is presented in Figure 4.1. The neutronics model of the benchmark is shown in Figure 4.2.
Figure 4.1: The PBMR400 Layout
The equilibrium core material definition is defined by giving number densities for 74 nuclides, two of which were not included in the models. These are $^{239}$U and $^{240}$Np. The reason for their exclusion is that the ENDF data for these two nuclides was not available in any of the evaluated nuclear databases. A list of all nuclides in the PBMR400 model is included in Appendix B.

A few adjustments were necessary to simplify the model for the purposes of method development for the determination of spectral zones. The 50cm helium gap between the bottom of top reflector and the top of the core was replaced with reflector material. The 12.5cm helium channel between the core barrel and the side reflector was
also replaced with reflector graphite material. Therefore the reflector dimensions were altered to the following new dimensions: the bottom reflector is 150cm, the top reflector is 200cm and the side reflector: 102.5cm which includes the 11.5cm control channel. The modified model is presented in Figure 4.3.

Figure 4.3: A Simplified PBMR400 Neutronics Model
4.4 MCNP Reference Results for the PBMR400 Core

The Monte Carlo N-Particle code MCNP5 (release 1.40) was used to generate a reference solution for the neutronics model of the PBMR400 design. The MCNP model was built as a combination of cylindrical and horizontal surfaces. The material number densities of the reflectors, control region and core barrel were used as provided in the benchmark specification.

The material specification of the fuel region was provided in 5 radial flow channels and 22 axial layers. The 5 radial channels were equally dimensioned into 17cm flow channels. Similarly the 22 axial layers were divided up into equally spaced mesh of 50cm. These channels were not necessarily selected on a particular zoning approach, but rather on intuition and experience of the reactor physicists involved in analyzing this reactor. Since the different material number densities between adjacent nodes introduce potential spectral effects, it was necessary to adjust the model and start with the simple case first. The model would then be improved at appropriate stages of the research to end up with a real complete model.

In the first MCNP model that was developed for this study, the 5 fuel region flow channels and 22 axial layers were homogenized into 1 material. This implies that for each radial flow channel, one set of material composition was used, instead of using 5 different material compositions in each channel. Similarly in the axial direction, no material variations were introduced in the 22 axial layers. The model was developed so as to match the model shown in Figure 4.3. The actual MCNP model contains more surfaces
for the detail that was necessary to define the solution. There are 141 radial surfaces and 58 axial surfaces in the model.

### 4.4.1 The Fuel Model

It is important to discuss the model of the fuel pebble used in this research. There are a number of approaches one can choose to model the PBMR fuel; the choice is essentially limited by the computational tool used. The fuel kernels inside the 5cm diameter fuel region can be modeled explicitly, with details of the TRISO layers, matrix material and the 0.5cm graphite shell. This model is generally known as the double heterogeneous model of the pebble fuel cell. The second option is referred to as the single heterogeneous model where all the materials of the fuel kernels are homogenized into one material. The third option is the homogeneous model where all fuel materials are homogenized into one material.

For this research the fuel pebble was not modeled heterogeneously as kernels with TRISO layers, but rather as a homogenized fuel model. One of the reasons for this approach is that the treatment of double heterogeneity of kernels in the pebble in MCNP is different to how it is treated in MICROX-2. This difference would introduce additional errors in the comparison of the two models. The intention in this work was to get as close and similar models between NEM and MCNP as possible. The approach in determining spectral zones is highly dependent upon the error between these two models. Therefore consistency between the two models (and minimal introduction of unquantifiable errors) was the major contributing factor for this choice.
Extensive research has been carried out on the comparison of the three models. It was shown that the effective multiplication factor is underestimated by 8% for the UO$_2$ homogenized fuel [25][26] compared to the double heterogeneous model. Kim et al [27][28] adopted a Reactivity-equivalent Physical Transformation (RPT) method to transform the double heterogeneity problem into a single heterogeneous one. The approach was shown to yield comparable $k_{\text{eff}}$.

The fluxes of the homogeneous fuel model would also be higher than those of the heterogeneous model. These differences are due to the fact that self-shielding is not properly accounted for in the homogeneous model. The heterogeneous and homogeneous models will be further investigated to establish the difference in the spectrum between the two models.

In this dissertation, the homogeneous core model is the one where the fuel material was homogenized into one material. The heterogeneous core model includes all 110 material compositions in the radial and axial dimensions.

4.4.2 Homogeneous Core at Uniform Temperature

The homogeneous model (all fuel materials homogenized into one material) of the PBMR400 core was developed and executed at three different temperatures: 800K, 1000K and 1200K. This is the temperature range of the fuel at normal operating conditions of the reactor. The effective multiplication factor $k_{\text{eff}}$ of the three cases is presented in Table 4.2. The absorption reaction rate, fission reaction rate, leakage rate and power density radial plots are shown in Figures 4.4, 4.5, 4.6 and 4.7 respectively. The 1000K graphs for the axial dimension are included in Appendix C. The radial power
density and radial fission reaction rate profiles are axially averaged over the core height. All other radial plots are axially averaged over the total height of the reactor. This applies to all radial plots presented in this dissertation. Axial profiles presented in this dissertation are averaged over the total radius of the reactor. Power density and fission reaction rate axial profiles are averaged over the core radius.

Table 4.2: MCNP $k_{\text{eff}}$ for the Homogeneous Core Model at 800K, 1000K and 1200K

<table>
<thead>
<tr>
<th>Temperature (K)</th>
<th>$k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>800K</td>
<td>$0.93729 \pm 0.00051$</td>
</tr>
<tr>
<td>1000K</td>
<td>$0.93293 \pm 0.00041$</td>
</tr>
<tr>
<td>1200K</td>
<td>$0.92488 \pm 0.00046$</td>
</tr>
</tbody>
</table>
Figure 4.4: MCNP Radial Absorption Reaction Rate for the Homogeneous Core
Figure 4.5: MCNP Radial Fission Reaction Rate for the Homogeneous Core

Figure 4.6: MCNP Radial Leakage Rate of the Homogeneous Core
4.4.3 Heterogeneous Core at Uniform Temperature

The heterogeneous case was developed based on the varying material densities in the 5 radial channels and 22 axial channels. Thus this case had 110 material sets in the core. As with the previous case, three temperatures were also considered for this case: 800K, 1000K and 1200K.

The comparison of the $k_{\text{eff}}$ for the 3 temperature cases is included in Table 4.3.
The radial absorption reaction rate, fission reaction rate, power density and leakage rate are plotted in Figures 4.8, 4.9, 4.10 and 4.11 respectively. Only the results of the 1000K are included in this section since the results do not differ much at other temperatures. Graphs of the axial dimension are included in Appendix D.

Table 4.3: MCNP $k_{eff}$ for the Heterogeneous Core Model at 800K, 1000K and 1200K

<table>
<thead>
<tr>
<th></th>
<th>$k_{eff}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>800K</td>
<td>$0.92881 \pm 0.00038$</td>
</tr>
<tr>
<td>1000K</td>
<td>$0.92430 \pm 0.00034$</td>
</tr>
<tr>
<td>1200K</td>
<td>$0.91635 \pm 0.00049$</td>
</tr>
</tbody>
</table>

Figure 4.8: MCNP Radial Absorption Reaction Rate of the Heterogeneous Core: 1000K
Figure 4.9: MCNP Radial Fission Reaction Rate of the Heterogeneous Core: 1000K

Figure 4.10: MCNP Radial Power Density of the Heterogeneous Core: 1000K
4.4.4 Heterogeneous Core with Actual Temperature Profile

The heterogeneous core model with 110 material number densities was further improved by applying the actual temperature profile of the core for the given set of equilibrium conditions. The models that have been developed thus far assumed uniform temperature in the core and reflectors. In reality, the core is not at uniform temperature. Thermal hydraulics codes are normally employed to perform heat and mass energy balances, and thereby determine the actual temperature profile in core. Depending on the model and the code used, the temperature profile would be determined node-wise in a spatial calculation mesh.
For the PBMR400 design, a temperature profile which was generated for the heterogeneous core using the VSOP code (as reported during the NEA/OECD benchmark meeting held on 21-25 January 2008) was used. The temperature profile in R-Z mesh is shown in Table 4.4. This mesh is based on the equally spaced 5 radial meshes (17cm each), and equally spaced 50cm axial meshes (22 meshes).

The radial absorption reaction rate, fission reaction rate, leakage rate and power density are plotted in Figures 4.12, 4.13, 4.14 and 4.15 respectively. Axial graphs are included in Appendix E.
Table 4.4: Actual R-Z Temperature Profile of the PBMR400 Core (K)

<p>| | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
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</thead>
<tbody>
<tr>
<td>830</td>
<td>818</td>
<td>810</td>
<td>802</td>
<td>798</td>
</tr>
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<td>861</td>
<td>844</td>
<td>831</td>
<td>822</td>
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<tr>
<td>911</td>
<td>887</td>
<td>872</td>
<td>861</td>
<td>858</td>
</tr>
<tr>
<td>967</td>
<td>940</td>
<td>925</td>
<td>920</td>
<td>925</td>
</tr>
<tr>
<td>1023</td>
<td>993</td>
<td>978</td>
<td>977</td>
<td>988</td>
</tr>
<tr>
<td>1072</td>
<td>1040</td>
<td>1024</td>
<td>1024</td>
<td>1036</td>
</tr>
<tr>
<td>1111</td>
<td>1079</td>
<td>1061</td>
<td>1062</td>
<td>1074</td>
</tr>
<tr>
<td>1141</td>
<td>1109</td>
<td>1091</td>
<td>1090</td>
<td>1101</td>
</tr>
<tr>
<td>1164</td>
<td>1132</td>
<td>1114</td>
<td>1112</td>
<td>1122</td>
</tr>
<tr>
<td>1181</td>
<td>1151</td>
<td>1132</td>
<td>1130</td>
<td>1137</td>
</tr>
<tr>
<td>1192</td>
<td>1164</td>
<td>1145</td>
<td>1142</td>
<td>1147</td>
</tr>
<tr>
<td>1200</td>
<td>1173</td>
<td>1155</td>
<td>1151</td>
<td>1155</td>
</tr>
<tr>
<td>1206</td>
<td>1180</td>
<td>1163</td>
<td>1157</td>
<td>1160</td>
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<tr>
<td>1210</td>
<td>1186</td>
<td>1168</td>
<td>1162</td>
<td>1164</td>
</tr>
<tr>
<td>1212</td>
<td>1190</td>
<td>1173</td>
<td>1166</td>
<td>1167</td>
</tr>
<tr>
<td>1214</td>
<td>1193</td>
<td>1176</td>
<td>1169</td>
<td>1168</td>
</tr>
<tr>
<td>1214</td>
<td>1195</td>
<td>1179</td>
<td>1171</td>
<td>1170</td>
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<tr>
<td>1214</td>
<td>1196</td>
<td>1180</td>
<td>1173</td>
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<tr>
<td>1214</td>
<td>1196</td>
<td>1182</td>
<td>1174</td>
<td>1171</td>
</tr>
<tr>
<td>1212</td>
<td>1196</td>
<td>1182</td>
<td>1174</td>
<td>1171</td>
</tr>
<tr>
<td>1210</td>
<td>1195</td>
<td>1182</td>
<td>1173</td>
<td>1170</td>
</tr>
<tr>
<td>1209</td>
<td>1195</td>
<td>1182</td>
<td>1173</td>
<td>1169</td>
</tr>
</tbody>
</table>
Figure 4.12: MCNP Radial Absorption Reaction Rate of the Heterogeneous Temperature Model

Figure 4.13: MCNP Radial Fission Reaction Rate of the Heterogeneous Temperature Model
Figure 4.14: MCNP Radial Power Density of the Heterogeneous Temperature Model

Figure 4.15: MCNP Radial Leakage Rate of the Heterogeneous Temperature Model
4.5 Conclusion

In this chapter, MCNP was identified as a transport code that produces the exact solution to particle transport because of its statistical nature, and also because every neutron is explicitly tracked. Thus the solution obtained from MCNP would be regarded as an exact reference solution.

The PBMR 400MW reactor is the selected PBR design for the development of spectral zones selection methodology. Three core configurations have been presented: the homogeneous core where all fuel materials were homogenized into one material, the heterogeneous core where 110 fuel materials in 5 radial channels and 22 axial nodes were used, and lastly the heterogeneous core with the actual temperature profile where the 110 materials were each assigned their actual temperature. In all these models the fuel pebbles were represented as a homogeneous material and no kernels or pebbles were modeled explicitly.

The results presented in this chapter form the basis of what would be referred to as the reference solution in this dissertation. Method development for determination of spectral zones is based on obtaining results that are as close as possible to the reference results presented here.
Chapter 5
Selection of the Energy Group Structure

5.1 Overview

One of the characteristics of graphite as a moderator in nuclear reactors is its low absorption cross section. In graphite neutrons scatter down to lower energies with a low probability of absorption. The slowing down of neutrons is highly dependant on the mass of the moderator. Of importance is the change in energy from the initial energy before scattering to the energy after the neutron has suffered a collision. Since graphite has a low average logarithmic energy decrement per collision compared to hydrogen as a moderator in Light Water Reactors, it follows that more collisions are necessary to slow the fast neutrons to thermal energies [7].

Multigroup equations are required to solve the diffusion equation for the graphite-moderated reactors. Two-group analyses have been shown to produce inaccurate results. Generally the minimum number of energy groups that have been used in practice for PBRs is four groups. Of great importance though, are the boundaries at which these group structures are defined. In solving the multigroup diffusion equation, the energy groups must be sufficiently narrow particularly in the thermal groups in order to properly account for upscattering. Also the thermal energy cutoff must be sufficiently high to prevent upscattering above this setting.
In this chapter, the importance of the correct group structure is discussed. The selection of the group structure used in this research is presented.

### 5.2 Theoretical Basis for a Proper Group Structure

The slowing down of neutrons is highly dependant on the atomic mass of the moderator [7]. Of importance is the energy change in scattering where the ratio of $E_2/E_1$ is defined by Eq. 5.1. $E_1$ is the initial energy before scattering and $E_2$ is the energy after scattering.

$$\frac{E_2}{E_1} = \frac{1}{2} [(1+\alpha) + (1-\alpha)\cos \theta]$$ \hspace{1cm} (5.1)

$$\alpha = \left(\frac{A-1}{A+1}\right)^2$$ \hspace{1cm} (5.2)

Eq. 5.2 defines alpha $\alpha$ which is calculated using the atomic mass of the moderator. For graphite, $\alpha = 0.716$; $\theta$ is the scattering angle of the neutron in the Laboratory system. It can be shown that the maximum energy loss in a collision will occur when the scattering angle is $\pi$, while the minimum loss of energy occurs when the scattering angle is zero. The minimum energy for a scattered neutron $E_{2,\text{min}}$ (when $\theta = \pi$) is given by Eq. 5.3.

$$E_{2,\text{min}} = E_1\alpha$$ \hspace{1cm} (5.3)
For hydrogen in LWRs $E_{2,\text{min}}$ is zero for all for all incident neutron energies. For graphite however $E_{2,\text{min}}$ is 0.716E$_1$. It is this property of hydrogen that enables two energy group analyses of water-moderated reactors, since many neutrons are scattered into the thermal group after only a few collisions with the moderator. The inability to do this in graphite is the reason for the need to perform multigroup analysis for graphite-moderated reactors.

Another contributing factor is that the resonance escape probability is considerably lower for graphite reactors (~ 8%) than LWRs. It takes many scatterings for a high energy neutron to pass through the resonance region on slowing down than in water where hydrogen can easily slow the neutron down past the resonance region in one collision. As neutrons slow down through the resonance region during many collisions there is greater probability that the neutron will be captured by resonance absorption than if it skips this process most of the time. In addition the neutron energy spectrum change is greater in the resonance region for graphite than in water. The higher temperatures in PBRs further harden the spectrum so that the reaction rates in the epithermal region are much higher than in LWR. Accurate modeling of these effects requires more than two energy groups.

The average logarithmic energy decrement per collision for graphite is 0.158; it takes about 114 collisions for the 2 MeV neutron to reach 0.0253 eV – compared with 18 in water moderated reactors [7].

The above discussion justifies the need for multi-group analysis for graphite-moderated reactors. For accurate multigroup analysis, proper thermal energy group
boundaries must be selected in order to accurately account for upscattering in the thermal energy range and the increased resonance absorption in the epithermal range. Additionally, the number of thermal groups and thermal group boundaries are very important for the low-lying plutonium resonances.

5.3 Existing Group Structures for PBRs

A sensitivity study was carried out to investigate the best group structures for the PBRs [19]. Several group structures were identified in this report together with the recommended group structures. The ideal approach to selecting a group structure for this research was to pick one of the recommended group structures identified in this report. However that was not possible for two reasons.

- As already indicated, diffusion cross sections are generated using a system of codes; NJOY, MICROR and MICROX-2. In MICROX-2 one of the limitations is that the cutoff energy for the point-wise resonance region calculations must be specified as one of the broad group boundaries. It would therefore be necessary to include this boundary in one of the recommended group structures. This approach worked well for some of the group structures.

- The investigation of the group structures identified in [19] was mainly carried out at 1000K. It emerged that some of the recommended group structures that worked very well at 1000K did not yield good results when applied to different temperature conditions of the core.
Since part of the scope of this research was to include investigations at different temperatures, it was necessary to establish a group structure that would yield sufficiently good results for the temperature range of interest. Therefore further investigations were necessary to identify a group structure that could be used for analyses at 800K, 1000K and 1200K.

5.4 The Temperature Effect on the Thermal Group Boundaries

In the slowing down of neutrons in a graphite-moderated reactor, fast neutrons experience collisions with the moderator and eventually reach thermal energies. It was explained in Section 5.2 that this would be after about 114 collisions. During the slowing down process in the fast groups, it is assumed that the effect of the thermal motion of the moderator is negligible. When the neutrons reach thermal energies, their energy is said to be in equilibrium with the thermal motion of the moderator atoms [7]. This thermodynamic equilibrium is characterized by a neutron spectrum that has a form of a Maxwellian distribution corresponding to the moderator temperature. It is at these low energies that the thermal motion of the moderator cannot be ignored. This implies that the neutron may gain energy based on the thermal motion of the moderator, and therefore upscattering has to be properly modeled.

The calculation of the scattering kernel depends on the selected model; free gas model or the crystal model. In both cases, the microscopic scattering cross section \( \sigma_s(E_1 \rightarrow E_2) \) is a function of temperature.
What makes this phenomenon so important are the low-lying plutonium resonances. Figures 5.1, 5.2 and 5.3 show the total cross sections of three of the plutonium isotopes as a function of energy. The figures were developed based on the General Atomics 193 fine group structure (see Appendix A). Evident from these graphs are the resonance peaks.

Figure 5.1: Pu239 Total Cross Sections versus Energy (eV)
Figure 5.2: Pu240 Total Cross Section versus Energy (eV)

Figure 5.3: Pu241 Total Cross Section versus Energy (eV)
A thermal boundary that was selected and found to be appropriate at one moderator temperature was identified as not appropriate at another temperature.

Upscattering in thermal groups occurs as a result of a neutron gaining energy following a collision with the moderator atom. Following such a collision, a neutron will then be scattered into a higher group. Carefully defined thermal boundaries would account for this event appropriately. With the low lying plutonium resonances, the effect of upscattering is significant and cannot be ignored. With an increase in the temperature of the moderator, the thermal motion of the atoms increases – the atoms would move faster at a higher temperature. The implication is that the neutron may gain even more energy after a collision with the moderator atom; hence the definition of the group boundaries around the plutonium resonances may no longer be appropriate for this changed condition.

5.5 Group Structure Selection

In selecting an appropriate group structure for NEM [23], the errors accrued for different multigroup structures were determined by evaluating the NEM results with the corresponding results of the MCNP reference solution presented in Chapter 4. The deviation of the NEM $k_{eff}$ from the reference $k_{eff}$ was tracked. For each boundary that was investigated, the group boundary that yielded the minimum deviation from the reference $k_{eff}$ was selected. Several group structures with various numbers of groups and boundaries were investigated.
A recommended group structure in [19] was selected as the starting point. The structure was adjusted by the addition of an appropriate group boundary for the point-wise resonance calculations in MICROX-2. The effectiveness of each boundary was tested at three temperatures (800K, 1000K and 1200K) by varying it with several of the boundaries from the 193-General Atomics group structure [14] [Appendix A]. A boundary that yielded the minimum deviation of $k_{\text{eff}}$ from the reference $k_{\text{eff}}$ was selected as a good boundary. The process was repeated for each of the boundaries in that particular group structure and for all temperatures.

The best boundaries from all three temperatures were combined into one structure. Duplicate boundaries were eliminated, and the boundaries that seemed close were combined. The reason behind this step was so that the final structure would not be too fine. The intention was to find the minimum possible number of energy groups without compromising accuracy, with six as the minimum number of groups allowed. In a similar manner, the effectiveness of each of the combined boundaries was investigated. The selection of the best boundaries was based on the boundary that yielded the lowest error in the $k_{\text{eff}}$ on comparison with MCNP reference $k_{\text{eff}}$.

This iterative process was followed until a reasonable 8-group, 10-group and 13-group structures were obtained. The details are discussed in the next sections.

5.6 Results

The fast group structures were established without difficulty. Structures based on 3-group and 6-group in the fast region were established, and proved to work well at all
three temperatures. For reasons already explained above, slowing down in the fast groups is not complicated by the thermal motion of the moderator, therefore upscattering in fast groups is not possible.

During the investigation to obtain the best thermal group structures, it was observed that the structure that was good for 1000K analyses was also somewhat acceptable for 1200K. However the 800K investigations based on the same group structure would always yield larger errors. Similarly, a structure that was good for 800K case, would not work very well for the other two temperatures, with the largest errors observed at 1200K (higher delta with 800K).

The reason for this observation is based on the proper selection of the energy boundaries that isolate the low-lying plutonium resonances for modeling upscattering. The boundaries that had the most influence in all three temperatures were 0.407 / 0.421 / 0.4325 eV, and 1.025 / 1.046 eV. These are the energy boundaries close to the 0.245 eV, 0.285 eV and 1.06 eV plutonium resonances (see Figures 5.1, 5.2 and 5.3). Irrespective of the number of groups in a selected group structure, a combination of these boundaries is what seemed to matter the most (the $k_{\text{eff}}$ was very sensitive to these boundaries). A combination that yielded the minimum $k_{\text{eff}}$ deviation from the reference at 800K was different to the one at 1000K and 1200K. Table 5.1 shows the best combination of these boundaries for each of the three temperatures based on an 8-group structure (other boundaries of a group structure are not included). The deviation from the reference $k_{\text{eff}}$ is also indicated.
It is important to note that according to the 193 group structure (see Appendix A), there is no other energy boundary in-between any of 0.407 / 0.421 / 0.4325 eV and 1.025 / 1.046 eV. Finding an optimum boundary outside of the 193 group structure was not an option because MICROX-2 is based on this structure, and therefore the boundaries of the broad group structure must be part of this fine group structure.

The identified trend in Table 5.1 is that the value of the energy boundary decreases with an increasing temperature. For example Boundary_A changes from 0.4325eV at 800K to 0.421eV at 1200K, and Boundary_B from 1.046eV to 1.025eV at 1200K.

Table 5.2 presents the best 8-group structure. This is based on the best combination of the boundaries identified in Table 5.1 such that the combined k\textsubscript{eff} deviation for all three temperatures is the minimum. This approach avoided a selection of the structure where a good agreement of the k\textsubscript{eff} at one temperature would yield the worst k\textsubscript{eff} deviation at another temperature. The deviation of the k\textsubscript{eff} for the three temperatures based on the best choice 8-group structure is shown in Table 5.3. This structure consists of 3 fast groups and 5 thermal groups.

<table>
<thead>
<tr>
<th></th>
<th>800K</th>
<th>1000K</th>
<th>1200K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_A</td>
<td>0.4325</td>
<td>0.4325</td>
<td>0.421</td>
</tr>
<tr>
<td>Boundary_B</td>
<td>1.046</td>
<td>1.025</td>
<td>1.025</td>
</tr>
<tr>
<td>k\textsubscript{eff} deviation</td>
<td>101 pcm</td>
<td>72 pcm</td>
<td>70pcm</td>
</tr>
</tbody>
</table>

Table 5.1: The Best Thermal Boundaries for 800K, 1000K and 1200K (eV)
The best 8-group structure identified in Table 5.2 is used in all analyses presented in this dissertation. It was found to yield acceptable reaction rate errors compared to the MCNP reference. The $k_{\text{eff}}$ deviation of 1000K and 1200K in Table 5.3 are relatively good. The 800K shows a higher deviation from reference MCNP $k_{\text{eff}}$; however this is still within an acceptable range. The groups structures presented in Table 5.4 and Table 5.5 were also found to be acceptable. However since the 8-group structure yielded good results, it was not necessary to choose a higher group structure.

**Table 5.2: The Best 8-Group Structure (eV)**

<table>
<thead>
<tr>
<th></th>
<th>FAST</th>
<th>THERMAL</th>
<th>THERMAL</th>
<th>THERMAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAST</td>
<td>1.49E+07</td>
<td>8.21E+05</td>
<td>7.102E+03</td>
<td>2.38</td>
</tr>
<tr>
<td>THERMAL</td>
<td>2.38</td>
<td>1.046</td>
<td>0.5285</td>
<td>0.407</td>
</tr>
</tbody>
</table>

**Table 5.3: $k_{\text{eff}}$ Deviation from MCNP Reference Based on the 8-Group Structure**

<table>
<thead>
<tr>
<th></th>
<th>800K</th>
<th>1000K</th>
<th>1200K</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_{\text{eff}}$ deviation</td>
<td>370 pcm</td>
<td>102 pcm</td>
<td>148pcm</td>
</tr>
</tbody>
</table>

The best 8-group structure identified in Table 5.2 is used in all analyses presented in this dissertation. It was found to yield acceptable reaction rate errors compared to the MCNP reference. The $k_{\text{eff}}$ deviation of 1000K and 1200K in Table 5.3 are relatively good. The 800K shows a higher deviation from reference MCNP $k_{\text{eff}}$, however this is still within an acceptable range. The groups structures presented in Table 5.4 and Table 5.5 were also found to be acceptable. However since the 8-group structure yielded good results, it was not necessary to choose a higher group structure.

**Table 5.4: The Best 10-Group Structure (eV)**

<table>
<thead>
<tr>
<th></th>
<th>FAST</th>
<th>THERMAL</th>
<th>THERMAL</th>
<th>THERMAL</th>
<th>THERMAL</th>
</tr>
</thead>
<tbody>
<tr>
<td>FAST</td>
<td>1.49E+07</td>
<td>8.21E+05</td>
<td>5.24E+04</td>
<td>9.12E+03</td>
<td>7.102E+03</td>
</tr>
<tr>
<td>THERMAL</td>
<td>2.38</td>
<td>1.025</td>
<td>0.5285</td>
<td>0.4325</td>
<td>0.12</td>
</tr>
</tbody>
</table>
5.7 Conclusion

It has been presented in this chapter that the graphite-moderated reactor requires more than two energy groups for accurate multi-group diffusion analyses. This is based on three phenomena:

The slowing down of neutrons in the graphite environment implies that a neutron would suffer several collisions before it reaches thermal energies. Energy group boundaries that would accurately model both down scattering and upscattering for the given problem must be defined.

The material composition (or burnup) of the fuel has an impact on the selection of appropriate energy group structures. The group structure needs to properly isolate important resonances. The PBMR400 equilibrium fuel definition has about 69 nuclides, including the isotopes of plutonium. The low lying resonances of Plutonium isotopes require a good thermal (finer) group structure. Analysis of the core using fresh fuel did not pose the challenges outlined in this chapter.

The temperature of the moderator also has an influence on the group structure. This was observed when a group structure that worked well at 1000K (and somewhat acceptable at 1200K) yielded inaccurate results at 800K. It was shown that the

<table>
<thead>
<tr>
<th></th>
<th>FAST</th>
<th>1.49E+07</th>
<th>8.21E+05</th>
<th>1.83E+05</th>
<th>5.24E+04</th>
<th>9.12E+03</th>
<th>7.102E+03</th>
<th>2.38</th>
</tr>
</thead>
<tbody>
<tr>
<td>THERMAL</td>
<td>2.38</td>
<td>1.6</td>
<td>1.025</td>
<td>0.5285</td>
<td>0.4325</td>
<td>0.12</td>
<td>0.04</td>
<td></td>
</tr>
</tbody>
</table>
differences observed as a result of the different moderator temperatures were influenced by the thermal motion of the moderator atoms. The speed at which the atoms move is a function of temperature; this thermal motion directly affects upscattering into higher energy groups. This directly impacted the upscattering modeling in the regions of low-lying plutonium resonances.

The 8-group structure was identified as the ideal group structure to use for this research for the PBMR analyses. It was selected based on comparisons of the $k_{\text{eff}}$ with the reference MCNP solutions at various temperatures.
Chapter 6
Spectral Zones Optimization Methodology

6.1 Definition of a Spectral Zone

A spectral zone is defined as a zone made up of a number of nodes whose characteristics are collectively similar and that are assigned the same few-group diffusion constants. It is a region over which the macroscopic and microscopic cross sections would be considered uniform for the purposes of a nodal diffusion core simulation or in other words it is a region over which the few-group spatial homogenization is performed.

The optimal selection of spectral zones based on the minimum number of zones would yield diffusion results within the specified accuracy when compared to a reference solution. Ideally the desired accuracy is retained for a one-to-one correspondence of zones with the nodes of a coarse mesh nodal diffusion model.

There are different approaches for analyzing the core in few-group diffusion theory with finite difference and nodal methods being the most well known and utilized. Both finite difference and nodal diffusion (to less extent since it is a higher-order method) algorithms become more accurate as the mesh is refined. Therefore refining the mesh to as fine as is allowed by numerical precision and computer memory would be ideal. There are two aspects of spatial mesh refinement to consider. The first is to obtain a spatially converged results for a given spectral zones selection. The second is to select the spectral zones based on spatial mesh refinement. The first aspect is a necessary study of any
discretization method (finite-difference or nodal) applied to a specific problem – the
provided solutions have to be spatially converged. The second aspect is an optimization
homogenization problem and is the subject of this research. Since the computational
efficiency is limited by available computer memory such optimization approach should
be a practical solution to the problem.

Optimum spectral zones strike a balance between accuracy and computational
efficiency. Properly defined spectral zones would allow for a higher-order model (such
as nodal method) with coarse mesh to yield results that compare close to a reference
transport solution, without the expense of fine mesh computational effort and generating
few group homogenized cross-sections for many meshes corresponding to the fine-mesh
discretization.

The impact that this research will have is to be able to give the ‘recipe’ for
dividing the core into zones that are physically representative, and to generate few-group
homogenized constants over these zones. This would yield the results with improved
accuracy without the burden of high computational effort and costs.

The best way of knowing if a zone size is fine enough is to check if there are
significant changes in the results if a finer zone size is used. It is important however to
ensure spatial mesh convergence (which depends on the discretization method used) of
the solution when optimizing spectral zone sizes. It is also important to keep in mind that
finer spectral zone sizes and finer computation mesh sizes (for selected zones) imply
higher computational costs in terms of storage and computational time.

In developing the method, the physics of what takes place in the reactor was
considered. Additionally, and more importantly, the heterogeneity of the reactor has been
considered. Generally, nuclear reactors are heterogeneous structures with multiple zones, including zones that contain fuels and zones that do not, as well as zones that contain control material. These have a huge impact on the behavior and the economy of neutrons in the core, and hence will affect the neutron spectrum and the choice of spectral zones.

6.2 Modern Equivalence Theory

In modeling the full heterogeneous reactor core using diffusion theory, the number of nodes used may be very large if all heterogeneous regions had to be represented. The PBMR 400 MW reactor (as defined in [3]) is physically heterogeneous, with a central reflector, side reflector, gas flow channels, and between the reflectors, a fuel zone comprising over 400,000 fuel pebbles of various burnup levels. If a diffusion code has to be used to analyze every heterogeneous detail, it will take several hundred thousand nodes to explicitly model the core. The computation time to solve this problem would be formidable and all likelihood not practical with current computational technology.

The widely used approach to addressing the above problem is to homogenize various regions of the core in such a manner that the diffusion theory parameters of the homogenized region are equivalent to the parameters of the heterogeneous region thus represented. This is the basis of Equivalence Theory [30] which was first developed for the homogenization of the fuel assemblies of light water reactors. This theory is based on the prescription that the three main parameters should be conserved. These are:

- The reactor eigenvalue, $k_{\text{eff}}$
• The node reaction rates (mainly fission and absorption)
• The surface currents/leakages across all surfaces of each node

The nuclear reactor engineer is mainly concerned with the balance of neutrons in the reactor. Hence special attention is paid to the creation of neutrons (fission), the destruction of neutrons (absorption) and the leakage into or out of the system.

All homogenized parameters in each node are assumed to be spatially constant. It is also assumed that the homogenization of the heterogeneous flux will preserve the surface currents between the nodes. For the heterogeneous case, the surface currents between adjacent nodes are assumed to be continuous, and so are the fluxes. It is therefore implied that the homogenized solution surface currents between adjacent nodes must also be continuous. Similarly one should think that the interface fluxes ought to be continuous. Whereas the former is found to be true (or enforced in the solution schemes), and thus the currents from the homogenized solution are continuous at boundaries, the latter cannot compatibly be enforced. That is, the fluxes from the homogenized solution can not be forced, and are generally not found, to be continuous. The advanced homogenization methods do not preserve the surface fluxes between adjacent nodes and allow for homogenized flux discontinuity as needed additional degree of freedom in the homogenization problem.

Koebke [30] suggested the use of heterogeneity factors. These are defined as the ratio of heterogeneous surface flux to homogeneous surface flux. He further imposed the restriction that the heterogeneity factors between adjacent nodes must be equal. This was necessary to conserve the homogeneous diffusion coefficient. Koebke’s findings are represented by the following equations as applied to fuel assemblies of LWRs [31][32]:
Since heterogeneous fluxes are continuous across the surface of each node:

\[
f_g^+ = \frac{\phi_g^+}{\hat{\phi}_g^+}
\]

(6.1)

\[
f_{g+1}^- = \frac{\phi_{g+1}^-}{\hat{\phi}_{g+1}^-}
\]

(6.2)

\[
f_g^+ = f_{g+1}^-
\]

(6.3)

Although Koebke’s new method was a ground-breaking tool for reactor physics, it suffered from the inefficiency of requiring an iterative update of the interface quantities.
This shortcoming was removed in the Generalized Modern Equivalence Theory introduced by Smith [31][32]. In Smith’s method all the information needed to produce continuous currents at interfaces and fluxes that are compatible with these currents are obtained at the homogenization stage and from the transport theory computations that are required for the said homogenization stage.

The method of Smith was later improved upon by Rahnema and Nichita [33]. They developed a technique to account for the inter-assembly neutron leakage effect on the homogenization parameters. This method brought about improvements in the nodal power accuracy for the heterogeneous models.

The widely used approach to addressing the above problem is to homogenize various regions of the core in such a manner that the diffusion theory parameters of the homogenized region are equivalent to the parameters of the heterogeneous region thus represented. In summary, a zone is equivalent to another if the reaction rates, the multiplication factor, and the leakage across all surfaces are equivalent. Thus, if these parameters based on diffusion theory are equivalent to the parameters of the heterogeneous transport solution, then the zones can be regarded as equivalent. These are the principles of Equivalence Theory that the research work presented in this dissertation respects.
6.3 Implicit Application of Equivalence Theory to Spectral Zones Determination

The preceding section describes how a heterogeneous reactor core can be homogenized in a manner by which reaction rates, group surface currents and the \( k_{\text{eff}} \) are preserved. This is achieved with a known heterogeneous solution (reference solution).

This same principle is applied in this research for determining the spectral zones for PBRs. The spectral zones are selected in such a manner that the diffusion parameters of each zone are preserved relative to the known reference solution. This is achieved by comparing the diffusion solution with the reference solution, zone-to-zone, and minimizing the error between the two by re-positioning zone boundaries of the diffusion problem.

Based on the findings in [31][32], it is important to preserve important group reaction rates (fission and absorption reaction rates), group surface currents and the \( k_{\text{eff}} \). In our investigation of determining spectral zones, the error to be minimized is the sum of the errors in each zone based on:

- Fission reaction rate error
- Absorption reaction rate error
- Net leakage across all surfaces of the zone

This error is determined using Eq. 6.6 and Eq. 6.7:

\[
\epsilon_{e_i,x} = \frac{\bar{\Sigma}_{\text{MCNP},x} - \bar{\Sigma}_{\text{NEM},x}}{\bar{\Sigma}_{\text{MCNP},x}} \times \frac{r_{i,i}^{2} - r_{-i}^{2}}{R_{h}^{2} - R_{o}^{2}}
\]  


(6.6)

\[
\epsilon_{\text{total}} = \sum_{x=1}^{3} \sum_{i=1}^{I} \epsilon_{e_i,x}
\]  


(6.7)
where:
\( \varepsilon_{\pm i,x} \) is the error of reaction type \( x \) in zone \( i \)
\( \bar{X}_{\text{MCNP},i} \) is the MCNP zone average reaction rate type \( x \) in zone \( i \)
\( \bar{X}_{\text{NEM},i} \) is the NEM zone average reaction rate type \( x \) in zone \( i \)
\( x \) is one of the three reaction types: leakage rate, fission or absorption reaction rates
\( r_{i-} \) and \( r_{i+} \) are the radial boundaries enclosing zone \( i \)

\( R_a \) and \( R_b \) are radial dimensions for the reactor region of interest. As an example, for optimization in the core \( R_a \) and \( R_b \) are 100cm and 185cm respectively for the 85cm PBMR400 core [2].

\( \varepsilon_{\text{total}} \) is the total error to be minimized base on all three reaction rates and all zones of the reactor region.

\( \varepsilon_{\pm i,x} \) is the error based on fission rate error, absorption rate error or the leakage, in each of the zones up to zone I. Therefore \( x \) represents: fission reaction rate, absorption reaction rate and the total current leakage (or in-leakage) at zone boundaries for in each zones.

The minimum error is achieved by implementing an optimization process to obtain the global minimum error of a function. The function as described in the previous paragraph is the sum of the errors in absorption reaction rate, fission reaction rate, and the currents for each node when compared against the reference solution. The detail of the optimization routine is addressed later in this chapter.

In an effort to ensure that leakages across the zones are preserved, an iterative process is performed to determine the appropriate diffusion coefficient. Thus, with each of optimization inner iterations it is necessary to recalculate the cross section and the diffusion coefficient for each of the zones.
6.4 Mean Free Path

The Mean Free Path (MFP) of a neutron is defined as the distance the neutron travels before it experiences a collision or interaction with a given type of nucleus [21]. It is an average distance traveled by a neutron between successive collisions. This distance is determined by the following function [20]:

\[
MFP = \frac{\int_0^{\infty} xe^{-\Sigma x} \Sigma dx}{\int_0^{\infty} e^{-\Sigma x} \Sigma dx} = \frac{1}{\Sigma}
\]

(6.8)

Where:

- \(x\) is a distance a neutron has succeeded to travel in penetrating the material without undergoing any interaction, and
- \(\Sigma\) is the macroscopic cross section of the reaction being considered.

The total mean free path includes all possible reactions: capture, fission and scattering. The concept of MFP is very important to this research. It has a huge impact on deciding how big or small the zones should be. Every attempt has to be made not to have zones that are too small relative to the MFP. If a zone is less than the MFP, it means the neutron can enter the zone, and simply pass to the next zone without experiencing any interaction. This will therefore introduce statistical errors in the solution and will not contribute much for reducing inaccuracies in solving the diffusion equation.

Another factor to consider with respect to spectral zones sizes is the fact that a spectral zone is defined based on a mixture of fuel spheres (or batches). Therefore to
make a spectral zones smaller and smaller, may result in a zone with the size of a fuel sphere. This would invalidate the assumption and definition of a spectral zone.

For the fresh pebble fuel, the average $\Sigma_t$ is about $0.22\text{cm}^{-1}$, resulting in a MFP of 4.5cm. For equilibrium fuel, $\Sigma_t$ is roughly $0.24\text{cm}^{-1}$, giving a MFP of about 4.2cm. In the reflectors, the MFP is about 2.3cm based on $\Sigma_t$ of $0.44\text{cm}^{-1}$.

For the purposes of this research, the limitation placed on the minimum zone dimension is two MFPs in the core. This constraint eliminates the possibility of having a zone that may be too small for practical purposes.

### 6.5 Choice of the Mesh or Zone Size

L Massimo [7] has looked into the aspects of choosing the mesh or zone size. These are useful items to consider, however they are very general and may not fit all reactor designs and computational methods (codes).

- The zone should be small where the flux is expected to vary rapidly.
- The zone size can be larger in regions of flat flux.
- The different zone sizes should vary smoothly.

Whereas these considerations are useful as a broad guideline, they should be refined further and applied in terms of a spectra rather than fluxes. That is, as is done in this work, the spatial variation of the spectrum rather than the fluxes should be the determining factor in choosing spectral zone extents. The best way of knowing if a zone size is fine enough is to check if there are significant changes in the results if a finer zone
size is used. More refined zone size means more computer storage capacity and computational time. Numerical difficulties can be encountered if the difference in the zone dimensions between adjacent zones is either too high or too low. The ratio in Eq. 6.9 need not be too large or too small; the size of zone $m$ must vary smoothly between adjacent zones $m-1$ and $m+1$.

\[
\frac{X_{m+1} - X_m}{X_m - X_{m-1}} \quad (6.9)
\]

Other factors will depend on the choice of the computer code and the method used. For instance some nodal codes may be very restrictive in terms of how one can vary the zone sizes.

6.6 Calculation of the Net Leakage Using NEM Currents

NEM produces a detailed output of the partial currents for the six different faces of a node. These are both outgoing and incoming partial currents. In cylindrical geometry, the net currents are calculated in the $r, \theta, z$ directions for each node. These are determined from Eq. 6.10 and Eq. 6.11 as follows:

\[
\begin{align*}
J_{r,+} &= J_{r,+}^{\text{out}} - J_{r,+}^{\text{in}} \\
J_{z,+} &= J_{z,+}^{\text{out}} - J_{z,+}^{\text{in}} \\
J_{\theta,+} &= J_{\theta,+}^{\text{out}} - J_{\theta,+}^{\text{in}}
\end{align*}
\] (6.10)
\[ J_{r,-} = -(J_{r,-}^{out} - J_{r,-}^{in}) \]
\[ J_{z,-} = -(J_{z,-}^{out} - J_{z,-}^{in}) \]
\[ J_{\theta,-} = -(J_{\theta,-}^{out} - J_{\theta,-}^{in}) \]  

\( J_{r,\pm}^{out}, J_{z,\pm}^{out}, J_{\theta,\pm}^{out} \) are partial outgoing currents in the \( r, z \) and \( \theta \) directions

\( J_{r,\pm}^{in}, J_{z,\pm}^{in}, J_{\theta,\pm}^{in} \) are partial incoming currents in the \( r, z \) and \( \theta \) directions

\( J_{r,\pm}, J_{z,\pm}, J_{\theta,\pm} \) are net \( r, z \) and \( \theta \) leakage terms in both directions

In two-dimensional cylindrical geometry, the net leakage is determined from the net currents using Eq. 6.12 and Eq. 6.13. The net currents are integrated over the volume of a node to determine the net leakage into or out of the node. The total leakage is the algebraic sum of the \( r \) and \( z \) net leakage terms indicated by Eq. 6.14.

\[ L_{r}^{net} = (J_{r,+} + J_{r,-}) \times 2 \pi r_i h_i \]  

\[ L_{z}^{net} = (J_{z,+} + J_{z,-}) \times \pi (r_{i+}^2 - r_{i-}^2) \]  

\[ L^{net} = -(L_{r}^{net} + L_{z}^{net}) \]  

\( L_{r}^{net} \) and \( L_{z}^{net} \) are the net leakage terms in the \( r \) and \( z \) dimensions.

\( r_i \) is the radius of node \( i \)

\( h_i \) is the height of the node \( i \)

\( r_{i+} \) and \( r_{i-} \) are the radial boundaries enclosing node \( i \).
The negative sign in Eq. 6.14 is based on the expression of the loss term in the diffusion equation (loss of neutrons). It is worth pointing out that the net leakage expressed by Eq. 6.14 is in units of \( \text{neutrons.s}^{-1} \). In order to obtain the rate in units of \( \text{neutrons.cm}^{-3}.\text{s}^{-1} \), the expression is divided by the zone volume.

With this approach outlined above it is possible to calculate all leakage terms for all zones in the \( r \) and \( z \) directions. The calculation of all leakage terms was incorporated into a script that optimizes the bucklings.

6.7 Leakage and Bucklings

In determining the balance of neutrons in a given volume, the time rate of change of the neutron density is equal to the production rate less the leakage rate, less the absorption rate. The equation for determining the net leakage rate can be derived using the net current densities. It is shown in [21] that the neutron leakage rate per unit volume in rectangular coordinates is derived and expressed by Eq. 6.15.

\[
\text{Net Leakage Rate} = -D\left(\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2}\right)
\]  

(6.15)

Using the Laplacian operator in rectangular coordinates, Eq. 6.15 can be simplified into Eq. 6.16

\[
\text{Net Leakage Rate} = -D\nabla^2 \phi
\]

(6.16)
The net leakage rate is calculated in units of number of neutrons per unit volume per second.

The bucklings are calculated using the data from NEM: the net currents, the zone fluxes and zone volumes. The currents from NEM are transformed into the net leakage term, \( L^{\text{net}} \) (using Eq. 6.14), which is equivalent to \( D \nabla^2 \phi \) in the diffusion equation, see Eq. 6.17.

\[
L^{\text{net}} = D \nabla^2 \phi \quad (6.17)
\]

It can be demonstrated that the term \( D \nabla^2 \phi \) is equivalent to \( DB^2 \phi \) \([21][22]\). The buckling \( B^2 \) is the unknown term. Therefore the bucklings can be determined by putting these parameters together as defined by Eq. 6.18

\[
B^2 = \frac{L^{\text{net}}}{D \phi} \quad (6.18)
\]

Where:

- \( L^{\text{net}} \) is the net leakage in \#n.cm\(^{-3}\).s\(^{-1}\)
- \( D \) is the diffusion coefficient in cm
- \( B^2 \) is the buckling in cm\(^{-2}\)
- \( \phi \) is the neutron flux in \#n.cm\(^{-2}\).s\(^{-1}\)

If \( L^{\text{net}} \) is expressed in \#n.s\(^{-1}\) then Eq. 6.18 should be divided by the volume.
Eq. 6.18 is for one group only. However group-dependent bucklings are necessary and are calculated using a similar equation with group fluxes, net leakage and diffusion coefficient, as shown in Eq. 6.19.

\[ B_g^2 = \frac{L_{g}^{\text{net}}}{D_g \phi_g} \]  

(6.19)

The process of calculating bucklings is an iterative process. The procedure starts with the initial bucklings supplied to MICROX-2. The initial estimates of the bucklings would typically be \(1 \times 10^{-10}\) for each of the energy groups (few groups, i.e. 8 groups). The few group generated cross sections are supplied to NEM. The partial currents are converted to groupwise net leakage terms, which are used together with the group fluxes, diffusion coefficients and zone volumes to calculate new groupwise bucklings using Eq. 6.18. The new few group buckling values are supplied to MICROX-2 and expanded to the fine group structure (193 groups). MICROX-2 is executed based on the new buckling values and new average diffusion constants are generated. The updated cross sections are passed to NEM, and new fluxes and partial currents are determined. The process is repeated until the convergence criterion is met. The convergence criterion that is used is the zone fluxes and the effective multiplication factor, \(k_{\text{eff}}\). The process is repeated until there is no significant change in the fluxes and \(k_{\text{eff}}\) between the current iteration and the previous one. This process is outlined in a flow diagram in Figure 6.1.
Figure 6.1: Process Flow Diagram for Optimization of Bucklings
6.8 Optimization of Spectral Boundaries

The identification of spectral boundaries is treated as an optimization problem which is solved by systematically and simultaneously repositioning all boundaries to achieve the global minimum error. The approach chosen was to optimize the core spectral boundaries in the radial dimension first, followed by the axial boundaries. Spectral boundaries in the reflectors were optimized last.

Various optimization techniques exist in solving optimization problems \[34][35][36]. The choices depend on various items like the nature of the function to be minimized, the constraints to be imposed, and whether parameters such as the derivative of a function can be determined.

For our optimization problem, the error to be minimized is the sum of the errors in each zone, calculated as a deviation or difference between the diffusion code results and the reference transport solution. As mentioned in the preceding sections, the three main parameters to be conserved are the reaction rates (fission and absorption), and the currents between the nodes, and the core multiplication factor.

The developed optimization algorithm performs the following steps:

- Given the user specified number of zone boundaries and the initial positions of these boundaries; the program calculates the average reaction rate in each zone for both the reference solution $\bar{x}_{MCNP}$ and the diffusion solution $\bar{x}_{NEM}$.
- From these averages, the program determines the error using Eq. 6.6 and Eq. 6.7. The total error is essentially the sum of the errors based on the
leakage, the fission and absorption reaction rates for each zone, averaged radially.

- The optimization subroutine is then called to minimize this error obtained above by systematically moving all boundaries, one at a time, to achieve the global minimum error.

The optimization scheme involves optimizing one boundary position at a time, starting from one chosen direction; say from left to right. When all boundaries have been re-positioned (first iteration), the process is re-started from the same initial direction with the first boundary. This process is followed until all the boundary positions cease to change. This is based on local optimization on the inner iteration and global optimization on the outer iteration.

To ensure that the important diffusion parameters are truly conserved, the cross section generation code is called at each of the inner iterations to re-calculate the cross sections and the diffusion coefficients, based on the newly suggested zone boundaries.

6.8.1 Optimization Process Flow

The optimization algorithm for identification of spectral zones is outlined in a step-by-step process below. This algorithm has been programmed and automated in a FORTRAN code [37].

a) Initial cross sections are generated with MICROX-2 based on all material specifications. The number of cross section sets matches the number of materials specified in NEM.
b) Spectral zones are determined in one reactor region at a given time. Thus the user specifies the core region, central reflector or side reflector as the region to optimize the spectral zones. The user also makes the choice of optimizing radially or axially. For the sake of clarity, the rest of this description focuses on radial optimization in the core. The procedure is however applicable in either dimension and for any reactor region that the user chooses.

c) The initial zone boundaries in NEM are arbitrarily selected. In this work, the initial state was always boundaries in equidistant positions. Thus for a 5-zone core region with an effective radius of 85cm, the 4 boundaries would be placed 17cm apart.

d) NEM is executed and the initial process of optimizing the buckling is started. This is the process described in Figure 6.1. The end of this iteration loop is a converged $k_{\text{eff}}$ and group fluxes.

e) The optimization procedure that has been developed is then called and optimizes one boundary at a time, starting from one chosen direction; say from left to right.

f) The positions of the first boundary are varied between two boundaries on either side of this first boundary. Refer to Figure 6.2 for the following illustration. The position of the first boundary $B_1$ is varied between $R_a$ and $B_2$. $R_a$ is an interface boundary between the central reflector and the core. A constraint on the minimum allowable zone size is included in the methodology based on discussions of mean free path in section 6.4. The minimum allowable zone size is 8cm. As a consequence, $B_1$ would be varied from $(R_a+8)$ to $(B_2-8)$, one centimeter at a time.
g) For each of the positions between (R_a+8) and (B_2-8), cross sections are updated and NEM is executed.

h) Using the output of NEM (group fluxes and net leakage for each zones), and the group diffusion data used to generate the NEM output, important reaction rates are calculated.

i) The objective function $\varepsilon_{total}$ is calculated as per Eq. 6.6 and Eq. 6.7 for all of the boundary cases identified in g) above.

j) A position that yields a minimum value for the objective function is selected as the new position for this boundary. A typical plot of $\varepsilon_{total}$ against radial positions is shown in Figure 6.3.
k) With boundary B₁ at its new position, Boundary B₂ is the next to optimize. The cross sections are updated and NEM is executed for all B₂ positions varied between (B₁+8) and (B₃-8). Reaction rates and the objective function are calculated. A position that yields a minimum value of the objective function is selected as the new position for B₂.

l) The process is repeated until all boundaries have been re-positioned (up to B₄ as per Figure 6.2). This would signal the end of the first iteration. The optimization
process is re-started from the same initial direction with the first boundary \( (B_1) \) for the second iteration.

m) This procedure is repeated until all the boundary positions cease to change. At that point, all boundaries would be globally optimized to define spectral boundaries.

The process described above is illustrated in Figure 6.4. The flow diagram summarizes the developed methodology. The next section presents the actual analyses that show the implementation of the procedure based on the PBMR 400MW design.
Figure 6.4: Process Flow Diagram for the Optimization Algorithm

- **Initial Input Bucklings**
- **MICROX-2**
- **NEM**
- Calculation of the net leakage
  - Group fluxes $k_{eff}$ Partial currents
  - $k_{eff}$ and flux tests
    - No significant change
    - Significant change in the fluxes and $k_{eff}$
    - New group bucklings
- **Optimum bucklings**
  - Test all possible boundary positions to obtain the minimum error
  - Select the optimum boundary
  - More boundaries to optimize?
    - Yes
    - More boundaries to optimize?
    - No
    - Compare all boundary positions with previous iteration
      - Different: Return for the outer iteration
      - No change
      - End of the outer iteration. Optimization process complete.
6.9 The PBMR400 Radial Spectral Zones

The optimization technique described in the previous section is applied to establish optimum spectral zones.

6.9.1 The MCNP Model

As described in Chapter 4, the MCNP models were developed for the purposes of establishing a reference solution for this research. The results that were presented define a reference solution for the different models described. The NEM models have been developed in a similar manner to the MCNP models to form the basis for comparisons.

6.9.2 The NEM Model

The NEM model is very similar to the model shown in Figure 6.5. The only difference is that the nodes are fewer.
100

### 6.9.3 Normalization of NEM and MCNP Sources

It was essential to have the NEM and MCNP normalized to the same source. The calculation of the fluxes and therefore reaction rates in both NEM and MCNP is dependent on the source strength. A minor deviation could have significant influence on the comparison and calculation of the error between the two codes.

<table>
<thead>
<tr>
<th></th>
<th>Graphite reflector</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>Control Channel</td>
</tr>
<tr>
<td>3</td>
<td>Core Barrel</td>
</tr>
<tr>
<td>4</td>
<td>Fuel region</td>
</tr>
</tbody>
</table>

**Figure 6.5: A Simplified PBMR400 Neutronics Model**
The MCNP Source

The MCNP source is calculated using Tally 7 using Eq. 6.20.

\[
\text{Total Reactor Power} = Source_{MCNP} \times \sum \text{power produced in all zones per unit source}_{Tally\,7}
\]

\[
Source_{MCNP} = \frac{\text{Total Reactor Power}}{\sum \text{power produced in all zones per unit source}_{Tally\,7}}
\] (6.20)

For the PBMR400 reactor, the total reactor power is 400MW. The output of tally 7 is in units of \(\text{MeV per fission per sec}\) for each power-producing cell. Each cell is multiplied by its mass to obtain \(\text{MeV per fission per sec}\). Adding this product for all the power-producing cells gives the total \(\text{MeV per fission per sec}\) for the reactor. The number of fissions per second (which is the source) can then be determined, given the total reactor power and the correct unit conversion factors.

NEM Source

The calculation for the NEM source is based on the recoverable energy, which is the energy released per fission. According to literature, the value of the recoverable energy ranges between 180 and 205 MeV per fission. This range is very wide and has proved to have a significant influence on the source calculations in Eq. 6.21.

\[
Source_{NEM} = \text{ReactorPower} \times Energy_{Recon} \times v
\] (6.21)
\( \nu \) is the number of neutron produced per fission. The recoverable energy should be units of \( \text{fissions/Watt.sec} \). With appropriate unit conversion factors, the number of fissions per second can be determined.

To ensure consistency between the NEM and MCNP sources, it is essential to use the same parameters in the calculations. As an example, the same value of the recoverable energy that MCNP uses, should be used for the NEM source. This value depends on the fissile isotopes present in the fuel. Based on the MCNP output for the equilibrium core, this value is about 184 MeV per fission.

### 6.9.4 Comparison of MCNP and NEM Models

As previously described, the statistical nature of the MCNP code makes it the best code to generate a reference solution. The code was used to generate the detailed reference solution for the simplified case of the PBMR400 model. The solution obtained here is compared with the NEM solution which was developed based on the equidistant zone boundaries (prior to optimization of spectral boundaries). To aid with development work for this research, the material number densities were homogenized both axially and radially into one material. This allowed for proper identification of spectral zones without the influence of material-based spectral boundaries. Later the results of the heterogeneous number density cases are also shown. Models for both MCNP and NEM were analyzed at 800K, 1000K and 1200K. The energy group structure used is the preferred 8-group structure. The comparisons included in this section are for the initial case based on 5 zones in the core. Therefore the 4 boundaries in the core are in equidistant positions; 17cm apart. Each of the five 17cm zones has 2 nodes (an assembly which comprises of
two nodes); therefore the graphs included in this section show the data points for each node.

<table>
<thead>
<tr>
<th></th>
<th>$k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCNP $k_{\text{eff}}$</td>
<td>0.93293 ± 0.00041</td>
</tr>
<tr>
<td>NEM $k_{\text{eff}}$</td>
<td>0.93388</td>
</tr>
<tr>
<td>Deviation from Reference</td>
<td>95 pcm</td>
</tr>
</tbody>
</table>

The effective multiplication factor is compared in Table 6.1. The deviation of NEM $k_{\text{eff}}$ from the reference is 95 pcm at 1000K.

A comparison of radially averaged absorption reaction rate, fission reaction rate, power density and the leakage rate are included in Figures 6.6, 6.7, 6.8 and 6.9 respectively. The plotted comparisons are for 1000K only; comparisons at 800K and 1200K are very similar and are therefore not included.
Figure 6.6: MCNP and NEM Absorption Reaction Rate at 1000K

Figure 6.7: MCNP and NEM Fission Reaction Rate at 1000K
Figure 6.8: MCNP and NEM Power Density at 1000K

Figure 6.9: MCNP and NEM Leakage Rate at 1000K
The net leakage plotted in the above graph is optimized as per the procedure outlined in section 6.7 and Figure 6.1. All the graphs indicate that there is a relatively good agreement between MCNP and NEM data, given the known limitations of few-group diffusion theory. The next section presents the optimized spectral zones, and their impact on the results already presented here.

6.9.5 Optimum Radial Spectral Zones

The results of optimized boundaries are presented. These were generated using the developed optimization algorithm already presented. To ensure that the important diffusion parameters are truly conserved, the cross section generation code is called at each of the inner iterations to re-calculate the cross sections and the diffusion coefficients, based on the newly suggested zone boundaries.

All radial boundaries in the reflectors and the axial boundaries were kept constant for the duration of the optimization process in the core.

The boundaries were optimized for 800K, 1000K, and 1200K. The number of zones in the core was varied from 5 zones as the initial case, up to 7 zones. For the 85cm effective radius of the core, the 100cm boundary and the 185cm boundary are the core/reflectors interfaces. Table 6.2 shows the boundaries of the optimized spectral zones together with the initial error and the final error ($\epsilon_{\text{total}}$) of the reaction rates. The actual dimension (size of each spectral zone) is shown in Table 6.3. The dimensions in all tables are in units of cm.
## 5-Zone Core

Table 6.2: Optimized Core Radial Spectral Boundaries: 5 Zones

<table>
<thead>
<tr>
<th></th>
<th>800K</th>
<th>1000K</th>
<th>1200K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_1</td>
<td>112</td>
<td>113</td>
<td>113</td>
</tr>
<tr>
<td>Boundary_2</td>
<td>127</td>
<td>129</td>
<td>128</td>
</tr>
<tr>
<td>Boundary_3</td>
<td>157</td>
<td>157</td>
<td>159</td>
</tr>
<tr>
<td>Boundary_4</td>
<td>173</td>
<td>175</td>
<td>173</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>Pre- Optimization</th>
<th>Post- Optimization</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCNP $k_{eff}$</td>
<td>0.93729 ± 0.00051</td>
<td>0.92488 ± 0.00046</td>
</tr>
<tr>
<td>NEM $k_{eff}$</td>
<td>0.940983</td>
<td>0.940825</td>
</tr>
<tr>
<td>$k_{eff}$ deviation</td>
<td>369pcm</td>
<td>354pcm</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>0.340099</td>
<td>0.277425</td>
</tr>
<tr>
<td>% Decrease in $\epsilon$</td>
<td>18.4%</td>
<td>20.6%</td>
</tr>
</tbody>
</table>
6-Zone Core

The results of the 6-zone core are presented below. Table 6.4 shows the boundaries of the optimized spectral zones together with the initial error and the final error ($\varepsilon_{\text{total}}$) of the reaction rates. The actual dimension (size of each spectral zone) is shown in Table 6.5.

Table 6.3: Optimized Core Radial Spectral Zone Dimensions: 5 Zones

<table>
<thead>
<tr>
<th></th>
<th>800K</th>
<th>1000K</th>
<th>1200K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spectral Zone_1</td>
<td>12</td>
<td>13</td>
<td>13</td>
</tr>
<tr>
<td>Spectral Zone_2</td>
<td>15</td>
<td>16</td>
<td>15</td>
</tr>
<tr>
<td>Spectral Zone_3</td>
<td>30</td>
<td>28</td>
<td>31</td>
</tr>
<tr>
<td>Spectral Zone_4</td>
<td>16</td>
<td>18</td>
<td>17</td>
</tr>
<tr>
<td>Spectral Zone_5</td>
<td>12</td>
<td>10</td>
<td>12</td>
</tr>
</tbody>
</table>
### Table 6.4: Optimized Core Radial Spectral Boundaries: 6 Zones

<table>
<thead>
<tr>
<th>Boundary</th>
<th>800K</th>
<th>1000K</th>
<th>1200K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_1</td>
<td>113</td>
<td>112</td>
<td>112</td>
</tr>
<tr>
<td>Boundary_2</td>
<td>123</td>
<td>123</td>
<td>123</td>
</tr>
<tr>
<td>Boundary_3</td>
<td>135</td>
<td>135</td>
<td>133</td>
</tr>
<tr>
<td>Boundary_4</td>
<td>156</td>
<td>155</td>
<td>158</td>
</tr>
<tr>
<td>Boundary_5</td>
<td>171</td>
<td>171</td>
<td>170</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th></th>
<th>800K</th>
<th>1000K</th>
<th>1200K</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCNP $k_{\text{eff}}$</td>
<td>0.93729</td>
<td>0.93293</td>
<td>0.92488</td>
</tr>
<tr>
<td></td>
<td>$\pm 0.00051$</td>
<td>$\pm 0.00041$</td>
<td>$\pm 0.00046$</td>
</tr>
</tbody>
</table>

#### Pre-Optimization

<table>
<thead>
<tr>
<th></th>
<th>800K</th>
<th>1000K</th>
<th>1200K</th>
</tr>
</thead>
<tbody>
<tr>
<td>NEM $k_{\text{eff}}$</td>
<td>0.940969</td>
<td>0.934028</td>
<td>0.923629</td>
</tr>
<tr>
<td>$k_{\text{eff}}$ deviation</td>
<td>368pcm</td>
<td>110pcm</td>
<td>125pcm</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>0.270514</td>
<td>0.248148</td>
<td>0.263331</td>
</tr>
</tbody>
</table>

#### Post-Optimization

<table>
<thead>
<tr>
<th></th>
<th>800K</th>
<th>1000K</th>
<th>1200K</th>
</tr>
</thead>
<tbody>
<tr>
<td>NEM $k_{\text{eff}}$</td>
<td>0.940946</td>
<td>0.933649</td>
<td>0.923614</td>
</tr>
<tr>
<td>$k_{\text{eff}}$ deviation</td>
<td>366pcm</td>
<td>72pcm</td>
<td>127pcm</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>0.250517</td>
<td>0.229345</td>
<td>0.230958</td>
</tr>
</tbody>
</table>

| % Decrease in $\epsilon$ | 7.4%  | 7.6%  | 12.3%  |
The results of the 7-zone core are presented below. Table 6.6 shows the boundaries of the optimized spectral zones boundaries together with the initial error and the final error ($\epsilon_{\text{total}}$) of the reaction rates. The actual dimension (size of each spectral zone) is shown in Table 6.7.

<table>
<thead>
<tr>
<th>Spectral Zone_1</th>
<th>800K</th>
<th>1000K</th>
<th>1200K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spectral Zone_2</td>
<td>10</td>
<td>11</td>
<td>11</td>
</tr>
<tr>
<td>Spectral Zone_3</td>
<td>12</td>
<td>12</td>
<td>10</td>
</tr>
<tr>
<td>Spectral Zone_4</td>
<td>21</td>
<td>20</td>
<td>25</td>
</tr>
<tr>
<td>Spectral Zone_5</td>
<td>15</td>
<td>16</td>
<td>12</td>
</tr>
<tr>
<td>Spectral Zone_6</td>
<td>14</td>
<td>14</td>
<td>15</td>
</tr>
</tbody>
</table>
Table 6.6: Optimized Core Radial Spectral Boundaries: 7 Zones

<table>
<thead>
<tr>
<th>Boundary</th>
<th>800K</th>
<th>1000K</th>
<th>1200K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_1</td>
<td>112</td>
<td>110</td>
<td>111</td>
</tr>
<tr>
<td>Boundary_2</td>
<td>120</td>
<td>120</td>
<td>120</td>
</tr>
<tr>
<td>Boundary_3</td>
<td>131</td>
<td>131</td>
<td>131</td>
</tr>
<tr>
<td>Boundary_4</td>
<td>152</td>
<td>155</td>
<td>150</td>
</tr>
<tr>
<td>Boundary_5</td>
<td>164</td>
<td>163</td>
<td>162</td>
</tr>
<tr>
<td>Boundary_6</td>
<td>176</td>
<td>175</td>
<td>173</td>
</tr>
</tbody>
</table>

| MCNP $k_{eff}$ | 0.93729 ±0.00051 | 0.93293 ±0.00041 | 0.92488 ±0.00046 |

<table>
<thead>
<tr>
<th>Pre- Optimization</th>
</tr>
</thead>
<tbody>
<tr>
<td>NEM $k_{eff}$</td>
</tr>
<tr>
<td>$k_{eff}$ deviation</td>
</tr>
<tr>
<td>$\varepsilon$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Post- Optimization</th>
</tr>
</thead>
<tbody>
<tr>
<td>NEM $k_{eff}$</td>
</tr>
<tr>
<td>$k_{eff}$ deviation</td>
</tr>
<tr>
<td>$\varepsilon$</td>
</tr>
</tbody>
</table>

% Decrease in $\varepsilon$: 7.7% 8.3% 3.9%
The results presented in the preceding tables indicate optimum spectral zones based on the 5-zone, 6-zone and 7-zone cores. It may seem that the 5-zone core is a better choice since it yields the greatest reduction in the error. Part of the reason is that the 6- and 7-zone cores have finer zone sizes as a result of the extra zone(s). Both finite difference and nodal diffusion (to a lesser extent since it is a higher-order method) algorithms become more accurate as the mesh is refined. Similarly one would expect the improvement in the error for a 5-zone core will be higher than that of a 6-zone core. The 7-zone core would have the lowest reduction in the error as it is evident from the results.

A detailed comparison of the 5-zone and 7-zone cases reveal the following detail (average boundary positions of the three temperatures are used in this discussion for simplicity as opposed to the actual boundaries specified in the tables):

- In the 5-zone case, the 128cm boundary is positioned as an optimum boundary between two spectral boundaries 120cm and 131cm as determined with the 7-zone core.

Table 6.7: Optimized Core Radial Spectral Zone Dimensions: 7 Zones

<table>
<thead>
<tr>
<th>Spectral Zone_1</th>
<th>800K</th>
<th>1000K</th>
<th>1200K</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spectral Zone_2</td>
<td>12</td>
<td>10</td>
<td>11</td>
</tr>
<tr>
<td>Spectral Zone_3</td>
<td>8</td>
<td>10</td>
<td>9</td>
</tr>
<tr>
<td>Spectral Zone_4</td>
<td>11</td>
<td>11</td>
<td>11</td>
</tr>
<tr>
<td>Spectral Zone_5</td>
<td>21</td>
<td>24</td>
<td>19</td>
</tr>
<tr>
<td>Spectral Zone_6</td>
<td>12</td>
<td>8</td>
<td>12</td>
</tr>
<tr>
<td>Spectral Zone_7</td>
<td>9</td>
<td>10</td>
<td>12</td>
</tr>
</tbody>
</table>
• This is confirmed by an additional zone (the 6-zone case) where the 120cm and the 131cm boundaries are identified as spectral boundaries, and the 128cm boundary is eliminated.

• Similarly the 157cm is an optimum boundary position between the 152cm and 163cm spectral boundaries obtained with the 7-zone core.

Discussions in Chapter 7 give further reasons why the 7-zone core identifies the best optimum spectral boundaries. Increasing the number of spectral zones beyond 7 does not yield significant improvement to the results.

6.10 Optimum Radial Spectral Boundaries with 5 Radial Material Zones

It was stated in earlier that the material number densities were homogenized over all zones to initially identify spectral zones without the additional spectral effects and mixing complexities introduced by varying material densities. In this section, the materials were varied into 5 radial channels averaged axially (materials were not varied axially). The number densities were specified according to the predetermined 17cm-zones.

A reasonable assumption that was made was that there would be an additional spectral boundary between each of the material boundaries. Therefore on top of the 117cm, 134cm, 151cm and 168cm material boundaries, five additional boundaries were placed equidistant between these boundaries. In Figure 6.10 the four material boundaries are indicated with the letter M and a subscript indicating the number of the boundary. The optimization routine was then executed to determine the optimum spectral boundaries for
B₁, B₂, B₃, B₄ and B₅ with the four material boundaries (M₁ to M₄) fixed. The results of the spectral boundaries are shown in Table 6.8. Material boundaries are indicated in bold since these were fixed and were not moved during the optimization process. These results are based on the 1000K case only.

Figure 6.10: A Heterogeneous Core with Additional Material Boundaries
The results in Table 6.8 reveal a very interesting similarity of the boundaries already determined and presented in Table 6.2 to Table 6.7 for the homogenized core. The only major difference is with the 143cm boundary. Of all the cases investigated thus far, there has been no boundary established between 134cm and 151cm boundaries. What is also of interest is the fact that this boundary is equidistant between the 134cm and 151cm boundaries. It is therefore not unreasonable to assume that this boundary is not necessarily a spectral boundary, but that it has been optimally positioned simply because it was defined as part of the problem under investigation. What supports this idea is the fact that the material number densities of channels 3 and 4 are not very different. A closer look at Figure 6.11 showing the fission reaction rate for this case in the radial dimension indicates that channels 2, 3 and 4 are very similar in composition where the graph is almost a smooth curve. The significant differences in the material number densities are evident with channel 1 and channel 5 (indicated by the step changes in the graph).

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Value (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_1</td>
<td>109</td>
</tr>
<tr>
<td>Boundary_2</td>
<td>117</td>
</tr>
<tr>
<td>Boundary_3</td>
<td>124</td>
</tr>
<tr>
<td>Boundary_4</td>
<td>134</td>
</tr>
<tr>
<td>Boundary_5</td>
<td>143</td>
</tr>
<tr>
<td>Boundary_6</td>
<td>151</td>
</tr>
<tr>
<td>Boundary_7</td>
<td>159</td>
</tr>
<tr>
<td>Boundary_8</td>
<td>168</td>
</tr>
<tr>
<td>Boundary_9</td>
<td>175</td>
</tr>
</tbody>
</table>
Therefore in light of this argument, the 143cm boundary is not expected to be a spectral boundary; however this must be confirmed with substantial evidence.

The observations discussed above led to the next investigation. The four spectral zone boundaries identified in Table 6.2 were used to adjust the 5-channel material model into a 5-spectral zones/material model. The given number densities in the five 17cm channels were adjusted or mixed (where necessary) to fit the dimensions of the spectral zones. Therefore the radial number densities were varied according to the defined spectral zones, and not by the equidistant 17cm zone model specified in the benchmark.

![MCNP Fission Reaction Rate for the Heterogeneous Core at 1000K](image)

**Figure 6.11: MCNP Fission Reaction Rate for the Heterogeneous Core**

The number densities in zones 2, 3 and 4 were recalculated based on the ratio of the volumes of these zones/materials to include the correct proportion of the adjacent material. The number densities in channels 1 and 5 were not altered. Figure 6.12
illustrates this new model, where previously defined material boundaries are indicated with dotted lines and the letter M with a subscript.

The first zone is made up of channel 1 material only. The second zone is a combination of the first and the second channel materials. The third zone is composed of material from channels 2, 3 and 4. Likewise the fourth zone has a portion of channels 4 and 5. Both MCNP and NEM were executed for this model and the $k_{\text{eff}}$ results are compared in Table 6.9. It would not be appropriate to compare the error of this case to that of the previous case with 9 spectral boundaries. The error in the former case would be much less because of the additional zones. That in fact drifts slightly off from what the intent of optimizing spectral boundaries is. The minimum possible number of spectral boundaries is determined in order to obtain reasonable results that compare well to the reference solution.

![Figure 6.12: A Model with number Densities Averaged Over the 5 Spectral Zones](image)
The spectral boundaries used in Table 6.9 were taken as average boundary results of the three temperatures as presented in Table 6.2. The results presented are for 1000K only. The important observation derived from the results of Table 6.9 is that the deviation of \( k_{\text{eff}} \) from MCNP reference is smaller when optimum spectral boundaries are used (as opposed to equally-dimensioned zones).

### 6.11 Discussion of Results

The results presented above identify spectral boundaries as those boundaries that minimize the error of the reaction rates in comparison with the reference MCNP reference results.
It can be seen that spectral boundaries agree to within ±2 cm for the three given temperatures. Each temperature case assumed uniform temperature in both the core and reflectors. This may imply that the spectral zones are not strongly influenced by temperature if there is no temperature gradient between the zones. The slowing down of neutrons, the resonances of important nuclides and the leakage between zones all have an influence on the characteristics of a spectral zone. These parameters are influenced by temperature. It is therefore to be expected that spectral boundaries will change somewhat when a realistic temperature profile of the PBMR core is applied to the model. This model is investigated in Chapter 10.

It was established during this study that the determination of spectral zones is highly influenced by the leakage between the zones. Therefore proper calculation of the leakage across zones was very important; hence the importance of the iteration process for optimizing group-dependent bucklings.

The energy group structure of choice has an influence on the identification of spectral zones. This became evident during the investigation when a 4-group structure yielded inconsistent results. Therefore a good group structure must be identified first before spectral boundaries can be properly identified. A good group structure will have characteristics of properly isolating and modeling important phenomena (such as resonances of important nuclides) in the core, based on the material composition of the fuel.

The results of the pre- and post-optimization error are sufficient proof that properly selected spectral zones yield results closer to the reference solution without the
increase in the computational effort that would result from the incorporation of an additional zone(s).

The 5-zone core shows the most improvement in the error when compared with the 6- and the 7-zone results. This was explained on the basis that the additional zones in the latter cases would, by the nature of nodal diffusion algorithms, yield a solution closer to the reference solution based on the increased number of zones.

The difference in the effective multiplication factor is to be expected. This is based on the fact that the fluxes from the MCNP reference solution are different from the diffusion-based fluxes, due to the limitations of diffusion theory. The effects of collapsing energy groups (from fine groups to broad groups) also contribute to the differences. Thus it has been observed that in some cases improvements in the reaction rates increase the $k_{\text{eff}}$ deviation from the reference slightly (only by a few pcm).

Thus far the methodology does not define the actual number of spectral zones that are required. The number of zones (and hence the number of spectral boundaries to be optimized) is specified by the user. The best number of spectral zones is determined by repeating the optimization process with one additional zone at a time. If the additional zone does not bring about the significant benefits of improved reaction rates, power distribution and the $k_{\text{eff}}$ versus the additional computational costs, then the previous case is regarded as having the best spectral boundaries.
6.12 Conclusion

A methodology for the optimization of spectral boundaries has been developed. The methodology is based on the principle of preservation of reaction rates and currents in each zone. This was achieved by comparing the diffusion solution based on NEM with the MCNP transport reference solution, and minimizing the error between the two solutions by repositioning the zone boundaries. This is essentially an optimization problem with the objective function for the optimization algorithm defined as the sum of fission, absorption and leakage rates errors between MCNP and NEM.

The leakage across the zones has been properly accounted for by defining an iterative loop for optimizing the group-dependent bucklings. This has proved to be an essential step in accounting for spectral effects of the adjacent zones.

The optimization algorithm developed during this research identified optimum spectral boundaries based on the 5-zone, 6-zone and 7-zone core. Significant improvement in the reaction rate errors were presented, with the biggest improvement obtained with the 5-zone core. The basis for this observation is that the diffusion algorithms yield improved solutions with additional zones (mesh refinement); thus the additional zones in the 6-zone and 7-zone models would yield a solution closer to the reference solution based on the increased number of zones.

The optimization methodology for identification of spectral zones was found to be consistent for the 3 temperature cases investigated. The 8-group structure also proved to be adequate for this methodology.
Chapter 7

Determination of Spectral Zones using Diffusion-Only Spectral Indices

7.1 Overview

The methodology that has been developed for the determination of spectral zones requires a transport reference solution. The optimization algorithm with the reference transport solution has proved to be accurate and consistent, however the computational effort required for completing the optimization process is significant. It was therefore necessary to develop a more practical methodology for the determination of the spectral zones in PBRs.

A spectral zone has been defined as a zone made up of a number of nodes whose material and spectral characteristics are collectively similar and that are assigned the same few-group diffusion constants. In other words the spectral zones are the regions over which the few-group diffusion parameters are generated for each spectral region.

The approach to this investigation was therefore to focus on the characteristics that define a spectral zone. These characteristics would be functions of the flux, reaction rates, currents, cross sections or even a combination of any of these parameters. The methodology would therefore involve the use of spectral indices based on few-group diffusion theory whole core calculations, without the use of a reference transport theory solution. The spectral index would define the characteristics of a zone such that when any
of the characteristics within a zone changes sufficiently, a new spectral boundary would be identified.

7.2 Spectral Indices

Several spectral indices were investigated. Special emphasis and focus was placed on the trend or behavior of the spectral index at various positions along the radial and axial dimension in the core. The following is a list of some of the spectral indices which were investigated:

- Fast to thermal flux ratio
- Group fluxes to total flux
- Epithermal flux to total flux ratio
- Epithermal to thermal $^{238}\text{U}$ captures
- Epithermal to thermal $^{235}\text{U}$ fissions
- $^{238}\text{U}/^{235}\text{U}$ fissions
- $^{238}\text{U}$ captures/$^{235}\text{U}$ fissions
- $^{238}\text{U}$ absorption to total cross sections
- $^{235}\text{U}$ fission/total cross sections

As much as each of the above spectral indices carry a particular meaning and detail regarding the phenomena occurring in the core, none showed a distinct change resulting from the changes in the spectrum. The two indices that were found to meet the criteria are:
• Groupwise surface currents to groupwise surface fluxes
• Groupwise surface currents to total surface fluxes

Special emphasis is placed on calculating these parameters at node surfaces and not within a node where volume-averaged parameters are calculated.

It was found that when the absolute value of these two ratios is plotted along the axial and radial dimension, the functions exhibit a series of minima and maxima points. The positions of these extreme points were found to correspond to the optimized spectral boundaries identified using the optimization tool and a reference transport solution. The details of the models used, results and comparisons are presented in the next sections.

The minima and maxima points of these spectral indices indicate a change in the gradient of the ratio; from an increasing function to a decreasing function, and vice versa. These points reflect a significant change in the spectral index (hence the change in the gradient of the curve). This supports the idea that a spectral zone is only defined as such while certain characteristics remain similar from node to node within that zone. At a node where a significant change occurs, the gradient of the ratio changes significantly, indicating a different set of conditions and therefore a new spectral zone. The spectral indices reflect the physical behaviors of interest which can be used to characterize behaviors within each zone and thus to identify and distinguish the spectral zones. This was shown to be a convenient method for the determination of spectral zones without the recourse to a reference transport solution.
7.3 The Derivation of Spectral Indices

Node surface fluxes and surface net currents are calculated using the surface partial currents defined in Section 6.6. Surface fluxes are defined by Eq. 7.1 and Eq. 7.2, while surface net currents are defined by Eq. 7.3 and Eq. 7.4.

\[
\phi_{g,(r,\theta,z)+} = 2\left(J_{g,(r,\theta,z)+}^{out} + J_{g,(r,\theta,z)+}^{in}\right)
\]

\[
\phi_{g,(r,\theta,z)-} = 2\left(J_{g,(r,\theta,z)-}^{out} + J_{g,(r,\theta,z)-}^{in}\right)
\]

\[
J_{g,(r,\theta,z)+} = (J_{g,(r,\theta,z)+}^{out} - J_{g,(r,\theta,z)+}^{in})
\]

\[
J_{g,(r,\theta,z)-} = (-1)\times(J_{g,(r,\theta,z)-}^{out} - J_{g,(r,\theta,z)-}^{in})
\]

The surface net currents will be named surface currents while surface partial currents will be named as partial currents in this text for sake of simplicity. Surface fluxes and surface currents were calculated in 2D \((r,z)\) only. The following description is based on the spectral index of groupwise surface currents to groupwise surface fluxes.

Based on the 8-group structure identified in Chapter 5, the 8-group spectral ratios are calculated as defined by Eq. 7.5. The ratios are calculated only on one side of the surface. For the radial dimension, for instance, the ratios are calculated either on the right side of the surface (+ direction) or on the left side of the surface (- direction), but not
both. This is because of the principle of continuity of fluxes and currents on either side of
the surface. Similarly, for the axial dimension the ratios would only be calculated either
on the top (+ direction) or bottom (- direction) of the node surface.

\[
\frac{|J_{1,(r,z)+}|}{\phi_1(r,z)+} ; \frac{|J_{2,(r,z)+}|}{\phi_2(r,z)+} ; \ldots ; \frac{|J_{8,(r,z)+}|}{\phi_8(r,z)+}
\]  \hspace{1cm} (7.5)

### 7.4 Plots of Spectral Indices for the Homogeneous Core

The spectral index of node surface currents to surfaces fluxes for the 8 energy
groups are plotted: the fast group ratios are plotted in Figure 7.1 and the thermal group
ratios are plotted in Figure 7.2. These graphs were generated based on the NEM model
for the homogeneous core at 1000K. The initial equidistant 17cm core zones (the 5 core
zones) were assumed in the model. It may be useful to also point out that each zone (for
which few group data is generated) is made up of a number of nodes. Thus the points
plotted in all the graphs are for the data calculated at each node surface.

The graphs of the 800K and 1200K reveal the same detail and are therefore not
included. Since the focus in this section is on the radial spectral zones, all the plots are
only for the core in the radial dimension, with the scale covering the core dimensions
only (100cm to 185cm). The spectral zone boundaries extracted from these plots is
compared to the results of a homogeneous core model obtained in Chapter 6 with the
reference transport solution.
As it has been stated, the minima and maxima points on these graphs indicate significant changes in the spectral ratio, where the gradient of the ratio changes from positive to negative, and vice versa. It is necessary to emphasize that the boundaries are defined only when the gradient of the ratio changes the sign. A small change in the spectral index that does not change the sign of its gradient is not a significant change to warrant a spectral boundary.

Since a spectral zone is characterized by the behavior of parameters in all energy groups within that spectral zone, if any group parameter changes significantly, that change warrants a spectral boundary. Hence the spectral boundaries in Figure 7.1 and Figure 7.2 are defined by different group ratios at different radial positions. The spectral boundaries identified from these figures are summarized in Table 7.1. These spectral boundaries are compared with reference spectral zone boundaries (based on the optimization procedure) in the next section.

<table>
<thead>
<tr>
<th>Spectral Index Boundaries</th>
<th>Identified by Group:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_A</td>
<td>106</td>
</tr>
<tr>
<td>Boundary_1</td>
<td>112</td>
</tr>
<tr>
<td>Boundary_2</td>
<td>121</td>
</tr>
<tr>
<td>Boundary_3</td>
<td>133</td>
</tr>
<tr>
<td>Boundary_4</td>
<td>152</td>
</tr>
<tr>
<td>Boundary_5</td>
<td>161</td>
</tr>
<tr>
<td>Boundary_6</td>
<td>176</td>
</tr>
</tbody>
</table>

Table 7.1: Core Radial Spectral Boundaries Based on the Spectral Index: Homogeneous Core at 1000K
Figure 7.1: The Ratio of Surface Currents-to-Fluxes for Fast Groups
Figure 7.2: The Ratio of Surface Currents-to-Fluxes for Thermal Groups
7.5 Comparison of Spectral Index with Reference Spectral Boundaries

The results of the 1000K homogeneous core obtained using the optimization routine and the transport reference solution are compared here with the spectral indices identified in the previous section.

With reference to Figure 7.1 and Figure 7.2, it emerged that the minimum and maximum points on these graphs correspond to the spectral boundaries determined using the optimization algorithm. The comparison of the two methods is shown in Table 7.2.

<table>
<thead>
<tr>
<th>Spectral Index Boundaries</th>
<th>7-Zone Optimized boundaries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_A</td>
<td>106</td>
</tr>
<tr>
<td>Boundary_1</td>
<td>112</td>
</tr>
<tr>
<td>Boundary_2</td>
<td>121</td>
</tr>
<tr>
<td>Boundary_3</td>
<td>133</td>
</tr>
<tr>
<td>Boundary_4</td>
<td>152</td>
</tr>
<tr>
<td>Boundary_5</td>
<td>161</td>
</tr>
<tr>
<td>Boundary_6</td>
<td>176</td>
</tr>
</tbody>
</table>

As it can be noted from Table 7.2 the results agree very well, except for the first boundary; Boundary_A. The reason for this discrepancy is based on one of the constraints imposed in the optimization routine. The smallest dimension allowed for a spectral zone was 8cm according to discussion of Mean Free Path in Chapter 6 (Section 6.4). Therefore a 6cm zone would not be identified by the optimization routine.
It is physically correct to have small boundaries adjacent to the core/reflector boundaries. The spectrum in the reflector is significantly different compared to the spectrum in the core; therefore the zones that are adjacent to the interfaces would experience different spectral effects. Additionally, the diffusion theory has some limitations and known discrepancies for modeling zones near interfaces. Therefore the largest errors in comparison with the reference transport solution are at the zones closest to the reflector/core interface. All group ratios show either a minima or maxima at the reflector/core interfaces; this confirms the big spectral differences at the core/reflector interfaces.

The spectral boundaries identified using the spectral indices are dependent on a choice of the energy group structure. It was emphasized in Chapter 5 that the group structure is very important especially for graphite-moderated cores based on slowing down theory. During the investigation of spectral indices, the 4-group structure yielded inconsistent results. The 6-group structure yielded good results but the accuracy of the boundaries was slightly reduced. The 10-group and 13-group structures yielded just as good and consistent results as the 8-group structure. The spectral index ratios of the 13-group structure are included in Appendix F.

The spectral indices are calculated at the surfaces of the nodes. Therefore one would expect that a finer mesh would identify the minima and maxima points (and therefore spectral boundaries) more accurately. Both fine mesh and coarse mesh cases were investigated. It was concluded that the mesh does not have to be too fine in order to identify accurate spectral boundaries.
An investigation was carried out to determine how the identified spectral boundaries would change if a core model is altered by representing the fuel region with only one material. Even though the previous case was based on a homogeneous model, few group diffusion data was generated for each zone. Thus, instead of using at least 5 fuel materials specified according to the 5 radial flow channels (17cm in size), only 1 fuel material for the whole 85cm core is used to define this model. This essentially defines the model as a one-zone core model with several nodes within this zone. NEM was executed and optimum bucklings were also determined for this case. The spectral index ratios of surface currents to surface fluxes are plotted and presented in Figures 7.3 and 7.4 for the 8 energy groups. The identified spectral boundaries are essentially identical to those which were identified in Section 7.4 above. The small differences in the graphs are due to the slightly coarser mesh sizes used for this model (5 nodes for every 17cm). The sizes of the core nodes in the previous section were smaller.
Figure 7.3: The Ratio of Surface Currents-to-Fluxes for Fast Groups: 1 Core Material
Figure 7.4: The Ratio of Surface Currents-to-Fluxes for Thermal Groups: 1 Core Material
7.6 A Core with Heterogeneous Number Densities

The heterogeneous core, which is characterized by the varying number densities in 5 radial channels and 22 axial nodes, is also investigated with the spectral indices. This is an important case to investigate since it contains all core material zones specified in the benchmark [3]. The surface current-to-flux spectral index is plotted for this case in three figures. Figure 7.5 shows the ratio for fast groups only; Figure 7.6 and Figure 7.7 shows the ratio for the thermal groups. The effects of the material discontinuities at the five material boundaries are immediately evident when compared to the homogenized material cases presented thus far.

The results extracted from the figures are presented in Table 7.3. These results are compared to the previous homogenized case in the same table (from Table 7.2). It can be noted that the 4 material boundaries (117cm, 134cm, 151cm, and 168cm) are identified as spectral boundaries in the figures. However additional boundaries are also evident from the graphs. The 4 spectral boundaries resulting from material boundaries are shown in bold in Table 7.3. The results indicate an interesting comparison with the homogenized case. Besides the spectral boundaries identified in bold in the table, the boundaries indicate some similarities and agree to ±2cm, except with the 161cm boundary.

It is important to note that the peaks defining spectral boundaries as a results of differences in the material number densities between the zones are not as sharp as the other minima and maxima points. The only minimum point that is both a material boundary and a significant spectral boundary is the 168cm boundary.
Figure 7.5: The Ratio of Surface Currents-to-Fluxes for Groups Fast Groups
Figure 7.6: The Ratio of Surface Currents-to-Fluxes for Thermal Groups 4 and 5
Figure 7.7: The Ratio of Surface Currents-to-Fluxes for Thermal Groups 6, 7 and 8
It is necessary to mention that the heterogeneous number densities in this model have introduced spectral shifts indicated by the shift in some of the boundaries. The boundaries have shifted an average of 3cm, with the largest shift on the 161cm/168cm boundary.

It is important to also highlight the fact that the second boundary was identified as 126cm (from group 1) and not 127cm (from group 4). Since these boundaries are very close one would think of a criterion for choosing either of the two boundaries. Unlike with the optimization algorithm where the optimum boundary would be automatically selected based on the minimum error in comparison with the reference solution, it is not an option in this case. However from the experience with optimization algorithm and detailed analyses of these boundaries and spectral ratios, in such a case the lower of the

<table>
<thead>
<tr>
<th>Spectral Boundaries for the Heterogeneous Core</th>
<th>Spectral Boundaries for the Homogenized Core</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_1</td>
<td>110</td>
</tr>
<tr>
<td></td>
<td><strong>117</strong></td>
</tr>
<tr>
<td>Boundary_2</td>
<td>126</td>
</tr>
<tr>
<td></td>
<td>121</td>
</tr>
<tr>
<td>Boundary_3</td>
<td><strong>134</strong></td>
</tr>
<tr>
<td></td>
<td>133</td>
</tr>
<tr>
<td></td>
<td>136</td>
</tr>
<tr>
<td>Boundary_4</td>
<td><strong>151</strong></td>
</tr>
<tr>
<td></td>
<td>152</td>
</tr>
<tr>
<td></td>
<td>154</td>
</tr>
<tr>
<td>Boundary_5</td>
<td><strong>168</strong></td>
</tr>
<tr>
<td></td>
<td>161</td>
</tr>
<tr>
<td>Boundary_6</td>
<td>178</td>
</tr>
<tr>
<td></td>
<td>176</td>
</tr>
</tbody>
</table>
two ratios is a better spectral boundary. A similar case exists with the 152cm and 154cm boundaries. The spectral ratio at 154cm (group 7) had a lower magnitude than the 152cm (group 8). The theory behind this observation is explained in the next section.

In light of the observations made thus far, the heterogeneous model (with the 17cm material boundaries) was altered to test the spectral index methodology further. Additionally, 10 or 11 spectral zones is a high number of spectral zones for the 85-cm core. Therefore the model was re-defined with the purpose to investigate the spectral boundaries of the heterogeneous case without the additional boundaries resulting from material boundaries. The material boundaries were altered to fit the identified 5-zone boundaries from Chapter 6. These boundaries are (average of the three temperature results) 113cm, 128cm, 157cm and 174cm. These boundaries agree very closely to the boundaries identified in Table 7.3 and were therefore used to adjust the material number densities into these zones as a starting point. The number densities in zones 2, 3 and 4 were recalculated based on the ratio of the volumes of these zones/materials to include the correct proportion of the adjacent material. Figure 7.8 illustrates this new model. Previously defined material boundaries are indicated with dotted lines. The M boundaries are the material boundaries in the original model, and the B boundaries are the spectral zone boundaries.

Keeping in mind that the B boundaries were developed for the homogenized case, this model was generated to determine the best spectral boundaries for the heterogeneous case, with the homogenized boundaries as a starting point. This was therefore done with the expectation that some differences in the spectral zones would be identified from the plot of the spectral ratios.
On plotting the spectral ratios following the model adjustments, the 152cm boundary consistently emerged as boundary. Therefore the model and number densities were adjusted accordingly to make the 152cm a boundary instead of the 158cm boundary. The 113cm boundary was also changed to 110cm since the spectral ratios consistently indicated this as a boundary. The graphs of the surface currents-to-surface fluxes ratio for this improved model are plotted in Figures 7.9, 7.10 and 7.11.

The spectral boundaries extracted from these above graphs are summarized in Table 7.4. These results represent the best spectral boundaries for the PBMR400 core.
Figure 7.9: The Ratio of Surface Currents-to-Fluxes for Fast Groups
Figure 7.10: The Ratio of Surface Currents-to-Fluxes for Thermal Groups 4 and 5
Figure 7.11: The Ratio of Surface Currents-to-Fluxes for Thermal Groups 6, 7 and 8
A balance had to be struck between two boundaries of 173cm and 176cm since these show from the graphs as boundaries. The 176cm boundary has a lower magnitude of the spectral ratio. Besides this fact, it would not be physically correct to define a new boundary 6cm from the 167cm boundary.

In Table 7.5 the spectral boundaries of the 7-zone homogenized core (presented in chapter 6) and the heterogeneous core are compared. As it can be noted from the table, the boundaries are in the same range, with the differences indicating the spectral changes due to the heterogeneous number densities introduced both axially and radially in the core.

These results also indicate that the approach of developing the methodology first with the simple homogenized core was a good approach. This made it possible to identify the appropriate number of spectral zones.

<table>
<thead>
<tr>
<th>Boundary_1</th>
<th>110</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_2</td>
<td>126</td>
</tr>
<tr>
<td>Boundary_3</td>
<td>135</td>
</tr>
<tr>
<td>Boundary_4</td>
<td>152</td>
</tr>
<tr>
<td>Boundary_5</td>
<td>167</td>
</tr>
<tr>
<td>Boundary_6</td>
<td>176</td>
</tr>
</tbody>
</table>
7.7 The Justification of the Spectral Index for the Identification of Spectral Boundaries

It was shown in Chapter 6 that the developed spectral zones optimization methodology yields good and consistent spectral boundaries. The spectral indices involving the surface currents also yield spectral boundaries that are consistent with the optimized boundaries. It is necessary to justify these observations based on the physics of this type of reactor.

In Chapter 6 it was shown how the currents calculated by NEM are converted into the net leakage terms to define the net leakage of a zone. The zone surface currents that are used to define the spectral index in this chapter are the same surface currents that are used to calculate the net leakage. An investigation of the surface currents and the net leakage across the zones revealed that the preferred spectral boundaries are at the surfaces where the net current of any energy group is zero or close to zero. Essentially
these would be at the surfaces where the net current changes direction, from a positive net current to a negative net current, and vice versa. This observation further emphasizes the importance of proper leakage representation for this reactor.

A detailed investigation of the properties of spectral zone boundaries revealed that the spectral boundaries were identified at the following points:

- All the minimum and maximum points of all group neutron sources (fluxes), neutron outscatter rates for fast neutrons, and fission rates for thermal neutrons.

- Points of inflection of the group fluxes (which occur close to the core/reflecter interfaces)

Figures 7.12, 7.13 and 7.14 show the radially averaged group surface fluxes generated with the NEM code, based on the homogeneous core model at 1000K. Special attention is drawn to the fluxes in the core region (between 100cm and 185cm), where the minimum and maximum flux points for each energy group are indicated on the graphs (with a black-shaded diamond). It is worthwhile to note that the fast and epithermal group fluxes have maximum points; and the thermal group fluxes have minimum points based on the flux shapes.
Figure 7.12: Homogeneous Core Group Surface Fluxes: Groups 1, 2 and 3
Figure 7.13: Homogeneous Core Group Surface Fluxes: Groups 4, 5 and 6
GROUP SURFACE FLUXES

Figure 7.14: Homogeneous Core Group Surface Fluxes: Groups 7 and 8
Mathematically, the minima and maxima points of a function correspond to the points where the derivative of a function is zero. Thus, the minima and maxima points of the surface fluxes would correspond to the points where the derivative of the flux is zero. This function (the derivative of the flux) would be represented by the neutron current density, as defined by Fick’s Law [22]:

$$J = -D \frac{d\phi}{dx}$$

Where:

- $J$ is the current density (#n.cm$^2$.s$^{-1}$)
- $D$ is the diffusion coefficient (cm)
- $\frac{d\phi}{dx}$ is the gradient of the flux relative to position in the x dimension

The first derivative of the group fluxes identifies spectral boundaries only at positions where the group currents are zero, and not the point(s) of inflection. Therefore positions where the second derivative of the flux (the gradient of the currents) is a minima or maxima, would identify all spectral boundaries, including those identified by the first derivative. These would be positions where the gradient is positive on one side of the boundary, and negative of the other side (and vice versa). Hence it is the gradient of the currents (the second derivative of the flux) that identify all spectral boundaries.

With reference to the 8-group structure, only one group flux profile had points of inflection; that is group 4. These points are identified in Figure 7.15 with a red diamond.
Figure 7.15: Homogeneous Core Group 4 Surface Flux with Inflection Points
Since it may be a little difficult to identify the points of inflection graphically using Figure 7.15, this point is further illustrated by Figure 7.16 which shows the graph of group 4 surface currents in the core only. The points of inflection are easily identifiable by the minimum and maximum points.

![GROUP 4 SURFACE CURRENTS](image)

**Figure 7.16: Homogeneous Core Surface Currents for Group 4**

It can be concluded therefore that the spectral boundaries are more likely to be identified at positions of zero currents. This implies that the flux is more isotropic at these boundaries.

The second important phenomenon is the slowing down of fast neutrons in graphite. In Chapter 5 the slowing down theory was presented as one of the important concepts for this type of reactor. Scattering of fast neutrons is much more pronounced
based on the fact that the neutron has to experience more collisions before reaching the thermal energy range. As it scatters and loses energy in the process, it moves from one group (the high energy group) to the lower group. As the neutrons scatter from one group to the next, they cross surfaces and leak into nodes where they contribute towards the flux in that node. The ratio of surface currents-to-surface fluxes is a parameter which defines how the current in a particular energy group changes relative to the flux in that group. It has been shown that the rate of change of this parameter shows a smooth increasing or decreasing trend from one surface to the next. This constant gradient is evident up to a point where the current changes direction. This change alters the ratio and causes significant change in the environment and therefore warrants a definition of a new environment. This is where the new spectral boundary is identified.

A decreasing magnitude of the surface current-to-surface flux ratio indicates that either the currents in that energy group are decreasing, or the fluxes are decreasing. As stated earlier, the preferred boundary is the one that exhibits lower currents; this explains why the boundary with the lower ratio is the preferred spectral boundary to any boundary in the vicinity that has higher currents.

The identified spectral boundaries, by definition, imply that the spectra within each spectral zone, is different to the spectra in the other spectral zones. To further illustrate this point, the Group-to-Total flux ratios plotted in Figure 7.17 shows the accrued Group-to-Total flux ratios. It can be seen in the core region of this graph that the ratio changes from one group to the next at the radial positions where spectral boundaries were identified (spectral boundaries not shown on this graph). The flux ratios with the
spectral boundaries are shown in Figure 7.18. These two graphs further confirm the validity of identified spectral boundaries.

Figure 7.17: Accrued Group-to-Total Flux Ratios
7.8 Conclusion

A practical spectral index has been defined that identifies spectral boundaries for the PBR core. The results based on this methodology compare very well with the optimized boundaries using the reference transport solution.

The results presented in this chapter confirm that the initial approach of developing the methodology based on homogenized core as an initial step was in fact a
very good approach. The best spectral boundaries for both the homogenized and heterogeneous cores are comparable, with differences due to the spectral shifts introduced by varying the material number densities in the core.

In Section 7.5 it was shown that the two models, one with 5 zones, and the other with 1 material zone, produced very similar spectral boundaries. This agreement of the spectral boundaries for the two cases is based on the understanding that zone boundaries are influenced by the scattering process (slowing down of the neutrons) and hence the leakage throughout the core. These boundaries occur where the spectral ratio reaches a minimum or maximum.

The ratio of the surface currents-to-surface fluxes plotted for all energy groups identify all spectral boundaries, thereby revealing the actual number of radial spectral zones for this core.

The spectral index approach does not eliminate the need to use the optimization algorithm with the reference transport solution. In fact the optimization approach is still a very good approach and is still recommended since it will identify the optimum boundaries even if fewer than needed zones are specified in the problem. This was observed with the results of the homogeneous case where 4 optimally positioned spectral boundaries yielded significant improvements to the results of a 5-zone core.
Chapter 8

Axial Spectral Zones Determination

8.1 Methodology

The methodology for determining radial spectral zones that has been developed and discussed in Chapter 6 was found to also be applicable to determining the axial spectral zones.

The challenge with axial zones is the initial computational effort required to optimize the zone boundaries over the 11m core. Nonetheless the method yielded consistent results. What is also of interest with the axial dimension for this reactor design is the fact that the control rods are inserted 150cm into the core (from the top of the core). As it was expected, this introduced significant spectral effects in this region of the core.

The optimization methodology with the transport reference solution was initially tested with the simple case where the number densities were uniform across the whole core. The great benefit to this simplification in the approach is the ability to isolate only the phenomena that influences the neutron spectrum (relative to the design and physical dimensions of the reactor) without additional spectral effects brought about by heterogeneous number densities. As it was shown in Chapter 7 the heterogeneous number densities bring about changes to the net leakage across surfaces, and therefore introduce spectral changes/effects. The dimensions of the core and reflectors as well as the presence
of control rods all have an impact on the identification of the spectral zones. The given number densities were therefore homogenized into one material.

The optimum axial spectral zones (optimized with the transport reference solution) were also confirmed using the spectral index as presented in Chapter 7. Once the methodology was validated for the axial spectral zones with the simplified homogenized case, the heterogeneous number densities were introduced to the model. This step was particularly important for the axial spectral zones because unlike with the radial number densities, the axial number densities differ significantly from the top to the bottom of the core. The fuel enters the core at top of the pebble bed, and is depleted as it moves through the 11m core. Therefore the average burnup of the fuel at the bottom of the core is higher as compared to the burnup of the fuel at the top of the core.

8.2 Calculation of the Error

Similarly to the radial spectral zones methodology, spectral zones are determined by minimizing the error between the MCNP reference solution and the diffusion solution (NEM). The error to be minimized is determined using Eq. 8.1 and Eq. 8.2

\[
E_{-i,x}^{+i} = \frac{|\bar{x}_{MCNP,x} - \bar{x}_{NEM,x}|}{\bar{x}_{MCNP,x}} \times \frac{\bar{h}_i}{\bar{H}_{core}} \quad (8.1)
\]

\[
E_{total} = \sum_{x=1}^{3} \sum_{i=1}^{f} E_{-i,x}^{+i} \quad (8.2)
\]
where:

$\epsilon_{i,x}^{+}$ is the error of reaction type $x$ in zone $i$

$\overline{x}_{MCNP,x}$ is the MCNP zone average reaction rate type $x$ in zone $i$

$\overline{x}_{NEM,x}$ is the NEM zone average reaction rate type $x$ in zone $i$

$x$ is one of the three reaction types; leakage, fission or absorption reaction rates

$h_i$ is the height of the zone

$H_{core}$ is the height of the core

It is necessary to include the ratio of the zone volume relative to the volume of the whole core so that the correct weighting is assigned to the error based on the size of the zone. Since for the axial zones, the radii are the same from zone to zone and only the height of the zone differs, the ratio of the volumes reduces to the ratio of the zone height to core height, as indicated by $h_i / H_{core}$ in Eq. 8.1.

### 8.3 Optimization Algorithm

The optimization procedure is carried out as follows:

- Given the user specified number of zone boundaries and the initial positions of these boundaries; the program calculates the average reaction rates in each zone for both the reference solution $\overline{x}_{MCNP}$ and the diffusion solution $\overline{x}_{NEM}$.
• From these averages, the program determines the error using Eq. 8.1 and Eq. 8.2. The total error is essentially the sum of the errors based on the leakage, the fission and absorption reaction rates, in all axial zones.

• The optimization subroutine is then called to minimize this error obtained above by systematically moving all boundaries, one at a time, to achieve the global minimum error.

The optimization scheme involves optimizing one boundary position at a time, starting from one chosen direction (usually from the top). When all boundaries have been re-positioned (first iteration), the process is re-started from the same initial direction with the first boundary. This process is followed until all the boundary positions cease to change.

Cross sections were generated with MICROX-2 based on all material specifications. The number of cross section sets matches the number of materials specified in the NEM input file.

The initial zone boundaries in NEM are placed in equidistant positions, with the necessary adjustment made to accommodate the position of the control rods. Since the control is inserted 150cm into the core, the 350cm boundary is regarded as a fixed boundary (200cm of the top reflector and the 150cm insertion depth).

For the control region, the initial assumption was that there would be 3 spectral zones in this region. The positions of the two boundaries to optimize were placed in equidistant positions. Following optimization of these boundaries, the third zone was added to the model to determine if the initial assumption of 3 zones was valid. The process was repeated for up to 5 spectral boundaries. The same optimization procedure as
described in Chapter 6 was implemented to determine the optimum positions of the spectral boundaries.

For optimization of radial zones in the core, each boundary was optimized by altering its position 1cm at a time, until the minimum error was achieved. In the case of axial zones, varying the boundary position 1cm at a time through the height of 1100cm would not constitute a practical approach. Therefore for the initial iteration, the boundaries were moved 10cm at a time. For the second iteration, the boundary was moved 3cm at a time to ±15cm of the position determined in the first iteration. In the third iteration, the boundary was altered every centimeter to ±5cm of the position determined in the second iteration. This way, the accuracy of the optimum position was not lost, and also fewer calculations were required to determine this optimum boundary position.

Several iterations were necessary to determine the number of boundaries to optimize over the 11m core. Also the inclusion of the control rods in the model added another dimension to problem. Part of the approach included optimizing the axial boundaries without the control rods in order to identify the average number of zones with and without control. 10 Zones were found to be more appropriate, hence it is the 10-zone results included in section 8.5.
8.4 Comparison of MCNP and NEM Models

The initial results of NEM are compared with the MCNP reference results prior to optimization. Comparisons are made based on the heterogeneous model where the number densities varied both radially and axially (110 fuel material sets).

The MCNP and NEM $k_{\text{eff}}$ are compared in Table 8.1. Reaction rates and the power density are compared in Figures 8.1, 8.2, 8.3 and 8.4. In the graphs, the region indicated as Control is the region up to which the control rod is inserted; this would be at 350cm from the top reflector for this core model.

<table>
<thead>
<tr>
<th></th>
<th>$k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCNP $k_{\text{eff}}$</td>
<td>0.92430 ± 0.00034</td>
</tr>
<tr>
<td>NEM $k_{\text{eff}}$</td>
<td>0.923988</td>
</tr>
<tr>
<td>Deviation from Reference</td>
<td>31.2 pcm</td>
</tr>
</tbody>
</table>
Figure 8.1: MCNP and NEM Axial Absorption Reaction Rate

Figure 8.2: MCNP and NEM Axial Fission Reaction Rate
Figure 8.3: MCNP and NEM Axial Power Density

Figure 8.4: MCNP and NEM Axial Leakage Rate
The differences noticeable from the graphs are expected and acceptable since a
diffusion code with its limitations, would not agree fully with MCNP-generated solution.
Hence the objective of optimally positioning zone boundaries so that the difference
between MCNP and NEM results (expressed as an error term $\varepsilon_{\text{total}}$ in Eq. 8.2) is
minimized. The two codes agree very well on the power density comparison.

8.5 Optimized Axial Spectral Boundaries for a Homogeneous Core

The results of optimized axial boundaries are presented in this section. These
were generated using the developed optimization algorithm. All radial boundaries in the
core and reflectors were kept constant for the duration of the optimization process in the
core axial dimension. The selected number of zones was 10 for the 11m core.

The optimum spectral boundaries for the homogeneous core together with the
initial error and the final error ($\varepsilon_{\text{total}}$) of the reaction rates are presented in Table 8.2. It is
useful to also give a view of the zone dimensions, as opposed to only showing the
boundaries. Table 8.3 presents the zone dimensions of the axial spectral zones for the
homogeneous core.
Table 8.2: Optimized Homogeneous Core Axial Spectral Boundaries: 10 Zones

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_1</td>
<td>216</td>
</tr>
<tr>
<td>Boundary_2</td>
<td>260</td>
</tr>
<tr>
<td>Boundary_3</td>
<td>280</td>
</tr>
<tr>
<td>Boundary_4</td>
<td>334</td>
</tr>
<tr>
<td>Boundary_5</td>
<td>350</td>
</tr>
<tr>
<td>Boundary_6</td>
<td>368</td>
</tr>
<tr>
<td>Boundary_7</td>
<td>850</td>
</tr>
<tr>
<td>Boundary_8</td>
<td>1268</td>
</tr>
<tr>
<td>Boundary_9</td>
<td>1286</td>
</tr>
</tbody>
</table>

**1000K**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Uncertainty</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCNP $k_{eff}$</td>
<td>0.93293</td>
<td>±0.00041</td>
</tr>
<tr>
<td>Pre- Optimization</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NEM $k_{eff}$</td>
<td>0.934028</td>
<td></td>
</tr>
<tr>
<td>$k_{eff}$ deviation</td>
<td>110pcm</td>
<td></td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>0.42087</td>
<td></td>
</tr>
<tr>
<td>Post- Optimization</td>
<td></td>
<td></td>
</tr>
<tr>
<td>NEM $k_{eff}$</td>
<td>0.934077</td>
<td></td>
</tr>
<tr>
<td>$k_{eff}$ deviation</td>
<td>115pcm</td>
<td></td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>0.40231</td>
<td></td>
</tr>
</tbody>
</table>

% Decrease in $\epsilon$ | 4.4% |
The spectral boundaries for this case were also determined using the spectral index methodology which was presented in Chapter 7. The spectral index of surface currents to total surface flux was used in this chapter. As previously mentioned, both spectral ratios reveal the same level of detail and therefore identify the same spectral boundaries.

The graphs of the spectral index in 8 energy groups are presented in Figures 8.5, 8.6, 8.7 and 8.8. These results are compared with the optimized boundaries in Table 8.4.

### Table 8.3: Optimized Homogeneous Core Axial Spectral Zone Dimensions

<table>
<thead>
<tr>
<th>Zone</th>
<th>Dimensions</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zone_1</td>
<td>16</td>
</tr>
<tr>
<td>Zone_2</td>
<td>44</td>
</tr>
<tr>
<td>Zone_3</td>
<td>20</td>
</tr>
<tr>
<td>Zone_4</td>
<td>54</td>
</tr>
<tr>
<td>Zone_5</td>
<td>16</td>
</tr>
<tr>
<td>Zone_6</td>
<td>500</td>
</tr>
<tr>
<td>Zone_7</td>
<td>18</td>
</tr>
<tr>
<td>Zone_8</td>
<td>418</td>
</tr>
<tr>
<td>Zone_9</td>
<td>17</td>
</tr>
<tr>
<td>Zone_10</td>
<td>15</td>
</tr>
</tbody>
</table>

The spectral boundaries for this case were also determined using the spectral index methodology which was presented in Chapter 7. The spectral index of surface currents to total surface flux was used in this chapter. As previously mentioned, both spectral ratios reveal the same level of detail and therefore identify the same spectral boundaries.

The graphs of the spectral index in 8 energy groups are presented in Figures 8.5, 8.6, 8.7 and 8.8. These results are compared with the optimized boundaries in Table 8.4.
Figure 8.5: The Spectral Index for the Homogeneous Core: Fast Groups

Figure 8.6: The Spectral Index for the Homogeneous Core: Groups 4 and 5
Figure 8.7: The Spectral Index for the Homogeneous Core: Groups 6

Figure 8.8: The Spectral Index for the Homogeneous Core: Groups 7 and 8
In comparing the spectral boundaries determined from the optimization methodology to those determined based on the spectral index (Table 8.4), it is evident that the two approaches yield comparable results. The differences are influenced by the fact that a 25cm mesh size was used in NEM. A finer mesh would certainly increase the accuracy of the spectral boundaries identified using the spectral index. However, this issue has to be analyzed in perspective; a 5cm improvement in the position of a boundary within an 1100cm core, is not worth the additional effort of mesh refinement, particularly if the benefit does not match the required effort.

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Optimized Boundaries</th>
<th>Spectral Index Boundaries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_1</td>
<td>216</td>
<td>225</td>
</tr>
<tr>
<td>Boundary_2</td>
<td>260</td>
<td>250</td>
</tr>
<tr>
<td>Boundary_3</td>
<td>280</td>
<td>275</td>
</tr>
<tr>
<td>Boundary_4</td>
<td>334</td>
<td>325</td>
</tr>
<tr>
<td><strong>Boundary_5</strong></td>
<td><strong>350</strong></td>
<td><strong>350</strong></td>
</tr>
<tr>
<td>Boundary_6</td>
<td>368</td>
<td>375</td>
</tr>
<tr>
<td>Boundary_7</td>
<td>850</td>
<td>850</td>
</tr>
<tr>
<td>Boundary_8</td>
<td>1268</td>
<td>1250</td>
</tr>
<tr>
<td>Boundary_9</td>
<td>1286</td>
<td>1275</td>
</tr>
</tbody>
</table>

Results obtained using both sets of results are in fact very comparable, with only 3pcm difference in the $k_{\text{eff}}$. It is also important to note that the optimized spectral
boundaries are accurate to ±2 cm since the boundaries were only altered in 2cm intervals for the last iteration during the optimization process.

An important observation made during the investigation of axial spectral zones is that the position of maximum flux (and maximum power density) is always identified as a boundary (see Figure 8.9). This is also the position where the net leakage changes the direction from a positive magnitude to a negative net leakage (the gradient of the flux).

Figure 8.9: NEM Axial Power Density for the Homogeneous Core at 1000K
8.6 Optimized Spectral Boundaries for the Heterogeneous Core

It was indicated at the beginning of the chapter that the homogenized model was necessary as the initial step in the process to identify spectral zones. This was necessary to confirm the application of the two methodologies to the axial dimension. The homogeneous model was then changed to include 110 materials in the core in 5 radial channels and 22 axial meshes.

Since the results of the optimized boundaries for the homogeneous case compared well with the results of the spectral index, this case was investigated only with the spectral index at 1000K using refined axial mesh. The optimum radial spectral zones determined in Chapter 7 were applied to the core model for this case.

The graphs of the surface current-to-surface flux ratio based on 8 energy groups are shown in Figure 8.10 for all 8 energy groups. All graphs show a very similar behavior compared to the homogeneous case, except for the ratio of group 1 which has additional details. Figure 8.11 shows the ratio of group 1 only for the discussions that follow.

The small peaks evident from the group 1 spectral ratio are a result of the varying material composition; varied every 50cm. These small peaks are similar to peaks that were also evident as a result of the heterogeneous radial number densities discussed in Chapter 7. The peaks are not large and distinctive such as those identified as spectral boundaries. Nonetheless they indicate spectral changes due to the varying material densities from one axial mesh to the next.
Figure 8.10: The Spectral Index for the Heterogeneous Core at 1000K – All Groups

Figure 8.11: The Spectral Index for the Heterogeneous Core in 1000K – Group 1
The boundaries identified by the group 1 spectral index are not included in the comparison. These are boundaries between 550cm and 1050cm at every 50cm. Since each of these zones is assigned a different material set, it is a given that each would be assigned its few group diffusion constants. Therefore this detail would not change or improve the model in any way.

The spectral boundaries extracted from Figure 8.10 are presented in Table 8.5 and compared with the homogeneous case. It was highlighted that one of the spectral boundaries is always identified at the position of axial maximum power density. For the heterogeneous case, the position of maximum power density is 550cm; see the power density graph plotted in Figure 8.3. The lower burnup at the top of the core (relative to the bottom of the core) is the cause for this shift in the peak power position. The homogeneous core with uniform material densities does not capture the effects of the varying burnup in the core; hence the peak power position would be located lower towards the middle of the core.

The spectral boundaries for the heterogeneous case identify one additional boundary at 338cm when compared to the homogeneous core spectral boundaries. This is a boundary between 325cm and 350cm. It is possible that this boundary existed with the homogeneous case but perhaps not as pronounced and could therefore not be detected with the coarse mesh plot of the spectral index. What is also observed is that the optimization routine identified the optimum position to be between these two boundaries at 334cm.
The differences in the 8th boundary are due to the position of axial maximum power density, which is 850cm for the homogeneous core and 550cm for the heterogeneous core. This shift in the peak is attributed to the appropriate assignment of the material number densities varied with burnup in the axial dimension. Since the burnup is lower at the top of the core when compared with the bottom core region, the peak power is expected to shift towards the top of the core.

The other differences in the spectral boundary positions are within the acceptable tolerance.
8.7 Discussion of Results

The optimization of spectral boundaries for the homogeneous case identified nine important spectral boundaries over the 11m core. In the region containing the control material, four spectral boundaries were identified. The spectral effects in this region are due to the effects of the top reflector, control material and the varying fuel number densities in the core. The remaining axial distance has only five spectral zones, with the first one close to the insertion point of the control rod. What is of importance to note is that the spectral zones in the remaining portion of the core are much larger, up to several centimeters close to the bottom reflector/core interface. Smaller zones near the bottom reflector/core interface are due to spectral changes influenced by the bottom reflector. Based on the detailed investigation of these boundaries, it was determined that the boundary between the two big zones is characterized by:

- The position of maximum power density and therefore the position of maximum axial flux
- The position where the net surface currents change from positive currents to negative currents

It was also observed that this position of maximum power density was identified as a spectral boundary for both the homogeneous and the heterogeneous core cases. During the investigation of other temperature models, the same observation was made.

The effects of the varying number densities in the axial dimension were observed with the spectral index of surface current-to-surface flux ratio of the first group, where material boundaries were identified as spectral boundaries. This effect is observed from
450cm to 1050 cm. In the first 150cm of the core it is not easy to make this observation because of the effects of the control material. For the same reason, 100cm beyond the control insertion level (up to 450cm), the effect of the varying material densities is insignificant because of the increased absorption rate due to the presence of $^{10}\text{B}$.

The reason for the observations of varying material densities in the first group is based on the following explanation. A high percentage of neutrons are born in this fast group as a result of fission. A change in the material number density (and in this case a reduction in the number density since the burnup increases axially from the top to the bottom of the core) influences the fission reaction rate and hence the rate at which neutrons are born. This change affects the flux, and hence the currents across surfaces in the same region. Therefore the ratio of surface currents-to-surface fluxes will show a sudden change in the ratio; in this case a peak at every surface where a change of material density is introduced.

It was also explained that the fuel pebbles are introduced into the PBMR core at the top of the pebble bed. The fuel moves through the core and it is removed at the bottom of the core through the de-fuelling chutes. As the fuel moves through the core, its burnup increases. This makes the fuel composition to differ significantly from the top to the bottom of the core. It is for this reason that the core would be made up of several material compositions within the 11m core. In light of this detail, the following is provided as the summary regarding axial spectral zones.

- Small spectral zones at surfaces adjacent to the interfaces: core/reflector/control insertion point are necessary. Results presented in this chapter indicate that about 10cm to 25cm are sufficient.
• Material boundaries would become spectral boundaries in dimensions selected in the depletion model. In this case, the material was varied every 50cm.

• The spectral effects introduced by the control rods make the insertion level (the 350cm boundary) a spectral boundary.

• The position of maximum axial power density is also a spectral boundary.

It can be concluded therefore that unlike with the radial spectral effects in the core, there are no major spectral effects in the axial dimension other than the varying material number densities. Small zones of about 10cm close to the reflector/control/core interfaces, and a spectral zone boundary at the position of maximum power density are the identified spectral zones. Since material number densities will differ in the axial dimension according to the specified depletion zones (50cm zones as it was observed with the PBMR400 model), it will be sufficient to treat these as spectral boundaries since few group diffusion data has to be supplied for each material zone. The mesh size within these zones would depend on the diffusion code used and on obtaining a spatially converged solution.

8.8 Conclusion

In this chapter, two methodologies have been presented for the determination of core spectral zones in the axial dimension. The approaches yield results that are comparable for both the homogenized core and the heterogeneous core. The following conclusions are drawn from the determination of axial spectral zones.
Small zones of about 10 to 25cm have been identified at all interfaces: reflector/core and core/control interfaces. A position of maximum power density is also identified as a spectral boundary. This is a position where the net leakage changes direction from positive net leakage to negative net leakage.

It was established that the axial spectral zones do not have a very big impact on the overall results. The reason is based on the fact that the material zones vary with the changing burnup from the top of the core to the bottom of the core. Since each material zone require its own few group diffusion data, this presents a fine axial structure that is not impacted by the defined spectral boundaries. For the PBMR400 core, number densities were supplies for every 50cm of the 11m core. A 25cm mesh yielded very good results. Three other mesh sizes of 10cm, 15cm and 20cm also gave good results. It can therefore be concluded that applying an axial grid structure of 25cm over the 50cm burnup zone is sufficient for this model. However it is important to ensure spatial convergence of the solution.
Chapter 9
Spectral Zones in the Reflectors

9.1 Overview

The relevant properties of the graphite reflector to reactor core neutronics have been identified in Chapter 2. It was shown that neutrons suffer several collisions in graphite before they are thermalized to lower energies. The important characteristic of graphite is its low absorption cross section which allows the neutron to scatter with the low probability of loss due to absorption. This accounts for the long diffusion length in graphite reflectors.

High energy neutrons leak from the core into the reflector where they are thermalized. Some will be lost due to absorption and leakage. However some will leak back into the core as thermal neutrons with the increased probability to be absorbed in the fuel to cause fission.

The neutron spectrum in the core (multiplying medium) is different from that in the reflector (non-multiplying medium). In this chapter the investigation was performed to identify spectral boundaries in the reflectors, and to determine their impact on diffusion core calculations.

Three regions of the reactor were excluded from the process of determining radial spectral zones in the reflectors. These are:

- The 11.5cm control channel
• The 7.95cm region in the side reflector located between the core and the control region

• The 5cm core barrel.

During this research, investigations were carried out at 800K, 1000K and 1200K. As with the other cases which have been presented thus far, the results for all three temperatures agree very well. It is therefore not necessary to include the results of all temperatures here. For consistency, only results of the 1000K are presented.

9.2 Methodology

Two reliable methods have been developed thus far in this research for identification of spectral zones. These two methods are tested and applied in this chapter in the determination of reflector spectral zones. The only difference introduced in the optimization methodology is the calculation of the error between the reference transport solution and the diffusion solution. Since the reflectors are non-fuel regions, there is no fission term in the calculation of the error. The total error was calculated based on the absorption and leakage rate errors.

The basis for using both methods is two-fold. It is necessary to confirm the results with two independent methods for verification purposes. It is also necessary to validate both methods for the reflector spectral zones since these two methods were developed and applied to the reactor core (neutron multiplying environment). The two methods were applied in the following manner:
• The spectral index of surface currents-to-surface fluxes was used to identify the number of spectral zones in the reflectors, and subsequently the spectral zone boundaries.

• Based on the identified number of spectral boundaries above, the optimization routine was executed to confirm the optimum positions of these boundaries.

This approach was implemented and applied to all four reflectors: central, side, top and bottom reflectors.

For the discussions that follow, it is necessary to present the group flux profiles of the heterogeneous model with emphasis on the reflectors. Figure 9.1 shows the graphs of all NEM-generated group fluxes in the radial dimension based on the 8-group structure. The fast fluxes in the reflectors are orders of magnitude lower than the thermal fluxes. Fast neutrons leak out of the core and scatter to thermal energies in the reflectors. The increase of thermal fluxes in the reflectors is due to slowing down of neutrons from fast energy groups. The thermal flux shows a maximum in the central and side reflectors a short distance from the core/reflector interface. This increase is due to the fact that fast neutrons are slowing down to thermal groups (thus increasing the thermal flux), and that the thermal neutrons are absorbed at a much lower rate in the reflectors compared to absorption in the fuel region. In the central reflector, most thermal neutrons are reflected back into the core. These would be absorbed in the fuel with the increased probability to cause fission. In the side reflector, the behavior is slightly different with the flux decreasing rapidly due to due to leakage (zero flux boundary condition).
The group flux profiles in the axial dimension are shown in Figure 9.2. For the same reasons given above, the fast fluxes are low in both the top and the bottom reflector compared to the thermal fluxes, however they also vanish rapidly towards the surface.

The above discussion explains why the spectra in the reflectors (non multiplying environment) would be different to the spectra in the core (neutron multiplying environment). The optimization algorithm was found to be applicable for the determination of spectral boundaries in the reflectors. A minimum error is obtained by repositioning each of the reflector boundaries.
The application and relevance of the current-to-flux spectral indices was investigated. It was found during the investigation that the surface current-to-surface total flux ratio yields more consistent results compared to the group-to-group current-to-flux ratio. The only differences between the two ratios were in the fast groups. Since the fast fluxes are lower in the reflectors, it is possible to identify a false peak in the ratio due to the lower fast flux (the lower value of the denominator in the ratio). The ratio of surface currents-to-total surface fluxes eliminates this potential error.

Figure 9.2: NEM Axial Fluxes for the Heterogeneous Core at 1000K
9.3 The Radial Spectral Zones in the Reflectors

The graphs of the spectral index of surface currents-to-total surface fluxes are presented in Figure 9.3 and Figure 9.4. Only the graphs of the thermal groups are included. The graphs of this spectral index in the fast groups do not show any minima or maxima points, therefore no spectral boundaries are defined by the fast group ratios. This observation implies that that the rate at which this spectral index changes from one radial surface to the next is either constant or it does not change significantly. The net currents in these fast groups do not change in direction.

![The Radial Spectral Index for the Central Reflector](image)

Figure 9.3: Radial Spectral Index in the Central Reflector: Groups 4, 5, and 6
The identified boundaries are compared in Table 9.1 with the boundaries obtained using the optimization algorithm.

**Table 9.1: Central Reflector Spectral Boundaries**

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Spectral Boundaries based on the Spectral Index</th>
<th>Optimized Spectral Boundaries</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_1</td>
<td>70</td>
<td>72</td>
</tr>
<tr>
<td>Boundary_2</td>
<td>80</td>
<td>84</td>
</tr>
<tr>
<td>Boundary_3</td>
<td>90</td>
<td>92</td>
</tr>
</tbody>
</table>
The results in Table 9.1 indicate that the most important boundaries in the central reflector are the ones closest to the core/reflector interface. This is the region where the changes in the spectrum are significant, where fast neutrons leak out of the core and thermal neutrons are reflected back into the core. This region is also characterized by positive and negative net leakages of various energy groups – a parameter which was found to influence spectral boundaries. This region is neutronically important; therefore the strong bias to have smaller spectral zones in this region is physically correct. Also comparison of reaction rates between the MCNP and NEM near the interfaces yields larger errors. This is because of the known limitation of diffusion theory near the interfaces. Thus smaller zones near the interfaces would reduce the error.

The initial error and final post-optimization error for the central reflector are presented in Table 9.2. The results do not yield a significant improvement in the $k_{\text{eff}}$. However a reduction of 11% in the reaction rate errors is significant. These results further confirm that the spectrum near the core/reflector interfaces is different to the spectrum several centimeters away; in this case up to 30cm away from this interface.

It is important to note that the proper definition of the mesh in the reflectors is very important for the diffusion code to yield accurate results. Improperly defined mesh sizes in the reflectors may yield inaccurate results. Thus the defined reflector spectral zones above do not eliminate the need for a proper mesh definition.

A test was conducted to determine if 5 spectral zones would be more appropriate for the central reflector. This was done by including an additional boundary to the above case. The fourth boundary was optimally positioned at 45cm. Further investigations of the error revealed that this additional boundary did not add much value in improving any
of the parameters. Therefore 3 spectral boundaries (4 zones) in the central reflector proved to be sufficient.

Table 9.2: Initial and Final Errors in the Central Reflector

<table>
<thead>
<tr>
<th></th>
<th>1000K</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCNP $k_{eff}$</td>
<td>0.92462 ±0.00060</td>
</tr>
<tr>
<td>Pre- Optimization</td>
<td></td>
</tr>
<tr>
<td>NEM $k_{eff}$</td>
<td>0.925775</td>
</tr>
<tr>
<td>$k_{eff}$ deviation</td>
<td>115.5pcm</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>0.20186</td>
</tr>
<tr>
<td>Post- Optimization</td>
<td></td>
</tr>
<tr>
<td>NEM $k_{eff}$</td>
<td>0.925758</td>
</tr>
<tr>
<td>$k_{eff}$ deviation</td>
<td>114pcm</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>0.17959</td>
</tr>
<tr>
<td>% Decrease in $\epsilon$</td>
<td>11.0%</td>
</tr>
</tbody>
</table>

The spectral index in the side reflector did not reveal any peak in any of the group plots. This was not at all surprising since both the thermal and fast fluxes in this region of the core vanish quiet rapidly. Nonetheless, the optimization routine was executed for positioning one boundary in the side reflector. It was expected that the boundary would be positioned close to the 204cm boundary where spectral effects are still significant. This was confirmed to be the case because in that region, the fluxes are still higher and are only starting to decrease rapidly. The boundary position was optimized at 216cm.
9.4 The Axial Spectral Zones in the Reflectors

The same approach identified in the above section was followed to determine the spectral zone boundaries in the top and bottom reflectors. It was established that 3 spectral zones were sufficient in both the top and bottom reflectors. The boundaries were identified close to the core\reflect interface. The results of the spectral ratio and optimized boundaries are compared in Table 9.3. The pre- and post-optimization errors are presented in Table 9.4.

<table>
<thead>
<tr>
<th>Spectral Boundaries based on the Spectral Index</th>
<th>Optimized Spectral Boundaries</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Top Reflector</strong></td>
<td></td>
</tr>
<tr>
<td>Boundary_1_1</td>
<td>175</td>
</tr>
<tr>
<td>Boundary_2_2</td>
<td>188</td>
</tr>
<tr>
<td><strong>Bottom Reflector</strong></td>
<td></td>
</tr>
<tr>
<td>Boundary_1_1</td>
<td>1313</td>
</tr>
<tr>
<td>Boundary_2_2</td>
<td>1325</td>
</tr>
</tbody>
</table>
9.5 Discussion of Results

The spectral boundaries in the top and bottom reflectors confirm once again that significant spectral effects are in locations close to the reflector/core interfaces. Based on the presented results in Table 9.3, two spectral zones of 10cm dimension would be appropriate in regions close to the interfaces in both the top and bottom reflectors. The results in Table 9.4 reveal a very small percentage in the improvement of the error. Two reasons justify this observation. The mesh size in the reflectors was already well defined (smaller nodes) prior to identification of spectral boundaries. This is based on the fact that improperly defined mesh size in the reflectors was found to yield inaccurate results
in NEM. Secondly, the errors in the top and bottom reflector are larger as the fluxes vanish rapidly towards the surface.

9.6 Conclusions

Two methodologies which were developed for determining spectral zones in the core were found to be relevant for the reflector spectral zones. The two methods have been shown to agree and yield spectral zones that are comparable.

It has been shown that for the reflectors in both the radial and axial dimensions, spectral boundaries are established close to the reflector/core interface. Spectral zones of 10 to 15cm have shown to be acceptable and yield reduced errors of the reaction rates. This improvement is also based on the fact that the error between the reference transport solution and the diffusion solution is high because of the limitations of diffusion theory at the interfaces. Therefore smaller spectral zones near the interfaces introduce significant improvement.

The results presented in this chapter and the observations made are summarized as follows:

- The changes in the spectrum at the reflector/core interfaces warrant small spectral zones at these interfaces.
- Spectral zones of 10cm to 15cm have proved to be sufficient for the top and bottom reflector. Three spectral zones in the top and bottom reflectors are good enough for this reactor. The fourth spectral zone was found not to
bring about any improvement in the results and was therefore not necessary.

- Two spectral zones in the side reflector were found to be sufficient since the fluxes in this region vanish quite rapidly. The improvement of reaction rates was not very great based on the same reason.

- Four spectral zones were established in the central reflector. The spectral boundaries of these zones were optimally positioned close to the reflector/core interface with an average dimension of 9cm. The central reflector was shown to be very important neutronically since it reflects most of the thermal neutrons back into the core.

It is important to note that the definition of the mesh in all reflectors is very important for the diffusion code to yield accurate results. Improperly defined mesh sizes in the reflectors were found to yield negative fluxes with the NEM code. Thus, the defined reflector spectral zones do not eliminate the need for proper definition of nodes dimensions in the reflectors. It is recommended to always verify spatial convergence of the diffusion solution.
Chapter 10

Application and Testing of Realistic Models

10.1 Introduction

The development of the methodology for identification of spectral zones for Pebble Bed Reactors was carried out using simplified reactor models. The basis for the simplifications was to have the ability to identify the spectral zones in an environment of limited spectral effects that could potentially complicate the development process. Thus temperature variations and material variations in the core were initially limited until the methodology was completely developed.

It is therefore appropriate to further investigate spectral effects and therefore spectral boundaries of more realistic core models. In this chapter two cases are investigated.

A realistic temperature profile of the PBMR400 core is applied instead of a model with uniform temperature. This is done using the heterogeneous number densities of the five radial channels and twenty two axial material meshes as defined in the model specification [3].

In all the models investigated, the control rods were inserted up to 350cm from the top of the top reflector (that is 150cm below the top of the core). The full insertion length of the control rods is 650cm below the bottom of the top reflector [3]. A new
model is developed where control rods are inserted to the 800cm from the top of the top reflector.

10.2 Heterogeneous Core with the Actual Temperature Profile

It has been shown in the previous chapters that the determination of spectral zones is not affected by the temperature at which the analyses are performed, when all material are at the same temperature. The spectral boundaries determined at 800K, 1000K and 1200K are essentially the same, with differences of ±2cm in a few of the boundaries.

In reality, the core is not at uniform temperature. Thermal hydraulics codes are employed to perform heat and mass energy balances, and thereby determine the actual temperature in core. Depending on the model and the code used, the temperature profile would be determined node-wise in a spatial calculation mesh, or zone-wise where several meshes make up the zone.

For the PBMR400 design, a fuel temperature profile which is based on the average of 9 participants of exercise 2 of the benchmark was used [39][40]. The temperatures vary by only a couple of degrees from one node to the next. For this reason, the values were rounded off to the nearest 10K. The temperature profile in R-Z mesh is shown in Table 10.1. Cross sections libraries for both MCNP and NEM were developed for 77 materials at 34 temperatures. MCNP and NEM models were developed for this case based on optimum spectral boundaries identified in the previous chapters for the heterogeneous model. A 5-zone radial core model was used. The temperature in all reflectors was assumed to be uniform at 1000K.
Table 10.1: Actual R-Z Temperature Profile of the PBMR400 Core (K)

<p>| | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
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<th></th>
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</thead>
<tbody>
<tr>
<td>830</td>
<td>818</td>
<td>810</td>
<td>802</td>
<td>798</td>
<td></td>
</tr>
<tr>
<td>861</td>
<td>844</td>
<td>831</td>
<td>822</td>
<td>818</td>
<td></td>
</tr>
<tr>
<td>911</td>
<td>887</td>
<td>872</td>
<td>861</td>
<td>858</td>
<td></td>
</tr>
<tr>
<td>967</td>
<td>940</td>
<td>925</td>
<td>920</td>
<td>925</td>
<td></td>
</tr>
<tr>
<td>1023</td>
<td>993</td>
<td>978</td>
<td>977</td>
<td>988</td>
<td></td>
</tr>
<tr>
<td>1072</td>
<td>1040</td>
<td>1024</td>
<td>1024</td>
<td>1036</td>
<td></td>
</tr>
<tr>
<td>1111</td>
<td>1079</td>
<td>1061</td>
<td>1062</td>
<td>1074</td>
<td></td>
</tr>
<tr>
<td>1141</td>
<td>1109</td>
<td>1091</td>
<td>1090</td>
<td>1101</td>
<td></td>
</tr>
<tr>
<td>1164</td>
<td>1132</td>
<td>1114</td>
<td>1112</td>
<td>1122</td>
<td></td>
</tr>
<tr>
<td>1181</td>
<td>1151</td>
<td>1132</td>
<td>1130</td>
<td>1137</td>
<td></td>
</tr>
<tr>
<td>1192</td>
<td>1164</td>
<td>1145</td>
<td>1142</td>
<td>1147</td>
<td></td>
</tr>
<tr>
<td>1200</td>
<td>1173</td>
<td>1155</td>
<td>1151</td>
<td>1155</td>
<td></td>
</tr>
<tr>
<td>1206</td>
<td>1180</td>
<td>1163</td>
<td>1157</td>
<td>1160</td>
<td></td>
</tr>
<tr>
<td>1210</td>
<td>1186</td>
<td>1168</td>
<td>1162</td>
<td>1164</td>
<td></td>
</tr>
<tr>
<td>1212</td>
<td>1190</td>
<td>1173</td>
<td>1166</td>
<td>1167</td>
<td></td>
</tr>
<tr>
<td>1214</td>
<td>1193</td>
<td>1176</td>
<td>1169</td>
<td>1168</td>
<td></td>
</tr>
<tr>
<td>1214</td>
<td>1195</td>
<td>1179</td>
<td>1171</td>
<td>1170</td>
<td></td>
</tr>
<tr>
<td>1214</td>
<td>1196</td>
<td>1180</td>
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<td>1171</td>
<td></td>
</tr>
<tr>
<td>1214</td>
<td>1196</td>
<td>1182</td>
<td>1174</td>
<td>1171</td>
<td></td>
</tr>
<tr>
<td>1212</td>
<td>1196</td>
<td>1182</td>
<td>1174</td>
<td>1171</td>
<td></td>
</tr>
<tr>
<td>1210</td>
<td>1195</td>
<td>1182</td>
<td>1173</td>
<td>1170</td>
<td></td>
</tr>
<tr>
<td>1209</td>
<td>1195</td>
<td>1182</td>
<td>1173</td>
<td>1169</td>
<td></td>
</tr>
</tbody>
</table>
The spectral index methodology was applied to determine the spectral zones. Radial spectral zones were determined first. The initial model was based on the 5-zone core radial spectral zones determined for the heterogeneous case at uniform temperature. These were 113cm, 128cm, 158cm and 175cm. Based on the results from this model, the material boundaries were adjusted to minimize their impact, and thereby minimizing the number of spectral zones to an optimum. The final spectral boundaries were obtained where material boundaries coincided with spectral boundaries. These new boundaries were used to adjust both the MCNP and NEM model for a proper comparison.

Table 10.2 shows the comparison of the $k_{\text{eff}}$ between NEM and MCNP based on the final spectral zones. A comparison of the spectral zones of the heterogeneous temperature model, the heterogeneous uniform temperature and the homogeneous uniform temperature models is presented in Table 10.3. The results in this table are for all identified spectral boundaries using the spectral index ratio of surface currents to surface fluxes.

### Table 10.2: MCNP and NEM $k_{\text{eff}}$ for the Heterogeneous Temperature Model

<table>
<thead>
<tr>
<th></th>
<th>$k_{\text{eff}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MCNP $k_{\text{eff}}$</td>
<td>0.91942 ± 0.00049</td>
</tr>
<tr>
<td>NEM $k_{\text{eff}}$</td>
<td>0.920033</td>
</tr>
<tr>
<td>Deviation from Reference</td>
<td>66.7 pcm</td>
</tr>
</tbody>
</table>
The results in Table 10.3 reveal a very interesting agreement of the results. This comparison indicates that the temperature in the core has minimal effect on the spectral zone boundaries. What is even more interesting is that the same spectral boundaries were obtained even for the homogeneous core model.

The comparison of the $k_{\text{eff}}$ of MCNP and NEM also shows a very good agreement; this is based on the small difference of 67pcm.

Axial spectral boundaries were also identified using the spectral ratio of surface currents to surface fluxes. As it was indicated previously, the material variation in the axial dimension is significant; therefore the model already defines this variation as a function of burnup. Nonetheless, the methodology was applied to identify the impact of temperature in the axial dimension.

On investigating the axial spectral index, it was revealed that the material boundaries were more pronounced not only in group 1, but also in the thermal groups.

<table>
<thead>
<tr>
<th>Boundary</th>
<th>Heterogeneous Core based on the Temperature Profile</th>
<th>Heterogeneous Core (1000K)</th>
<th>Homogenized Core (1000K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boundary_1</td>
<td>110</td>
<td>110</td>
<td>112</td>
</tr>
<tr>
<td>Boundary_2</td>
<td>123</td>
<td>126</td>
<td>123</td>
</tr>
<tr>
<td>Boundary_3</td>
<td>135</td>
<td>135</td>
<td>135</td>
</tr>
<tr>
<td>Boundary_4</td>
<td>153</td>
<td>152</td>
<td>155</td>
</tr>
<tr>
<td>Boundary_5</td>
<td>166</td>
<td>167</td>
<td>163</td>
</tr>
<tr>
<td>Boundary_6</td>
<td>176</td>
<td>176</td>
<td>175</td>
</tr>
</tbody>
</table>

Table 10.3: Comparison of the Radial 7-Zone Temperature Model Spectral Boundaries with the Homogenized and Heterogeneous Core Models
There was no additional detail in the epithermal groups. With the previous uniform temperature core model, it was only group 1 that identified material boundaries. There is no other significant difference between this model and the uniform temperature core model. This outcome further supports what was presented in Chapter 8; that the axial dimension requires a proper axial grid or mesh structure to properly account for the varying material densities with burnup.

10.3 Movement of Control Rods

A model was developed where control rods were inserted up to 800cm from the top of top reflector. This new model was based on the heterogeneous case with the temperature profile. It was expected that inserting control rods deeper into the core would introduce significant spectral effects to this model.

The spectral index of surface currents to surface fluxes was used for the identification of spectral boundaries. The plots of the spectral index for all energy groups show a significant change to the spectral boundaries in both the axial and the radial dimensions. Both radial and axial plots of the spectral index are included from Figure 10.1 to Figure 10.6. The axial power density is shown in Figure 10.7; it also shows some interesting details regarding the position of the control rods.
Figure 10.1: The Radial Spectral Index for Control Model – Fast Groups
Figure 10.2: The Radial Spectral Index for Control Model – Groups 4 and 5
Figure 10.3: The Radial Spectral Index for Control Model – Groups 6, 7 and 8
Figure 10.4: The Axial Spectral Index for Control Model – Fast Groups
Figure 10.5: The Axial Spectral Index for Control Model – Groups 4, 5 and 6
Figure 10.6: The Axial Spectral Index for Control Model – Groups 7 and 8
The plots of the spectral index reveal that there are significant spectral changes in both the radial and axial dimensions as a result of the insertion of control rods to 800cm. This is a significant change to the spectra particularly in the axial dimension. The peak power (and maximum flux) positions shows a shift towards the bottom of the core at 1075cm. This is an expected outcome for a control rod insertion.

The axial spectral index graphs also reveal the peaks corresponding to the variation of material number densities. This trend was already identified in Chapter 8. All the axial graphs also reveal a spectral boundary at about 1075cm; which corresponds to
the peak power position and maximum flux position. This also confirms the observation made with the other models in previous chapters.

Radially there are minor spectral boundary shifts of ±3cm. The spectral index of group 6 may appear to have a slightly different shape; however it reveals the same detail as with the other heterogeneous cases.

10.4 Conclusion

The analysis of the temperature model presented in this chapter confirmed that the temperature variation in the core does not have a significant impact on the spectral zone boundaries. This conclusion is made based on the good agreement of spectral boundaries for the three different models:

- Homogeneous core model
- Heterogeneous core model
- Heterogeneous core model with the actual temperature profile

It is further concluded that the consistency of the spectral boundaries with temperature variations indicate that an appropriate group structure was used in the model. Further analysis of the axial spectral index has confirmed that the properly selected axial mesh is sufficient to model the burnup variation in the axial dimension.

The control rod model was a good test that revealed that the spectral index of surface currents to surface fluxes responds appropriately to significant changes in the spectra. The results presented are in line with the expected spectral shifts.
The test cases presented in this chapter further extend the application of this methodology for various core models. This validates the methodology presented in this dissertation.
Chapter 11
Conclusions and Recommendations for Future Work

11.1 Conclusions

The objective of this research was to develop a methodology for determining optimum spectral zones for the Pebble Bed Reactor. An optimization methodology has been developed to optimally position PBR spectral zone boundaries thereby reducing the error between MCNP reference solution and the nodal diffusion code NEM. This is achieved without increasing computational costs for obtaining the NEM diffusion solution. Using the optimal spectral zones, selected 8 energy groups, and appropriate axial mesh, the NEM calculated power distribution and $k_{eff}$ for the equilibrium core are sufficiently precise to perform design calculations. A thermal hydraulics code can perform accurate temperature calculations using the NEM power distributions.

It has also been shown that spectral zones can be automatically identified using diffusion theory data only. The spectral index of surface currents to surface fluxes exhibits a series of minima and maxima points when plotted against the radial and axial dimensions of the reactor. These minima and maxima points correspond to the optimum spectral zone boundaries.

It is necessary to mention that the identified optimum spectral zones would not lead to a complete agreement between the transport reference solution and the diffusion solution. The limitations of diffusion theory would always result in the differences
between the two approaches (diffusion theory and transport theory). Thus the optimum spectral zones yield a diffusion solution that is closer to the references transport solution as compared to the diffusion solution where optimal spectral zones were not used in the model. Using optimal spectral zones has been shown to give sufficiently close agreement to MCNP reference solution to enable NEM to be a design code for PBRs.

The contributions in this dissertation are summarized as follows:

11.1.1 MCNP Reference Model

Optimizing various input parameters in NEM together with the development of the methodology for determining spectral zones required a transport reference solution. MCNP5 was chosen as the transport code for this purpose. MCNP generates an exact transport solution based on its stochastic nature. Thus different reactor core models based on the PBMR 400MW reactor design were created and analyzed using MCNP to create accurate reference solutions. These formed the basis for optimization comparative analysis. The NEM diffusion theory solutions were compared with MCNP reference results for the identification of spectral zones.

The MCNP reference solutions were also utilized to determine the best energy group structure for this research. Optimum group boundaries were selected based on the $k_{\text{eff}}$ comparison between MCNP and NEM. The best boundaries were those that yielded the minimum $k_{\text{eff}}$ deviation from the reference solution.

As a consequence the optimized input structure of the selected 8 energy groups and 5 optimized spectral regions resulted in a NEM model yielding value of $k_{\text{eff}}$ with a
deviation of 0.0010 (100 pcm) of reference Monte Carlo prediction. The power distribution was exact when compared with MCNP. Thus this work provides an excellent model for NEM to perform design calculations for the PBR.

11.1.2 Cross Section Generation

It has been demonstrated that the use of proper tools for generating cross sections is very important. NJOY, MICROR and MICROX-2 were shown to be an adequate cross section generating system of codes for performing diffusion theory calculations with NEM. NJOY was also used to generate continuous energy cross sections for MCNP at various temperatures based on the procedure which was outlined in this dissertation. The procedure was validated by comparing a core model analyzed with built-in MCNP cross sections at 293K, to the model where new cross sections were used. A comparison of the $k_{eff}$ showed a very good agreement between the two cases, with a difference of 0.0023%. Cross sections generated with the tools described in this dissertation have been shown to be adequate for this research.

11.1.3 Selection of the Broad Energy Group Structure

Special characteristics of graphite-moderated reactors were identified with emphasis to justify the need for multigroup diffusion analyses. It was shown that unlike the water-moderated reactors where hydrogen is the moderator, the fast neutron has to experience many collisions in graphite before reaching thermal energies and attain
thermal equilibrium with the moderator atoms. Properly defined thermal group boundaries were shown to be of utmost importance in modeling upscattering particularly in the presence of low-lying plutonium resonances.

The temperature in the core also has an influence on the thermal group structure. This was observed when a group structure that worked well at 1000K and 1200K yielded inaccurate results at 800K. It was shown that the differences observed as a result of the different moderator temperatures were influenced by the thermal motion of the moderator atoms. The speed at which the atoms move increases with an increase in temperature. Thus at higher temperatures the moderators atoms move faster thereby increasing the probability of upscattering of the neutron to a higher energy group. This directly impacted the upscattering modeling in the regions of low-lying plutonium resonances. Increasing the number of carefully selected energy groups in order to model correctly all of the relevant physical phenomena decreases the impact of temperatures on the deviations between diffusion and Monte Carlo solutions towards spectral converged diffusion solutions.

The 8-group structure consisting of three fast groups and 5 thermal groups was identified as the ideal group structure to use for this research for the PBMR analyses. Thermal boundaries in the region of the plutonium resonances were carefully selected in such a manner that the deviation of the effective multiplication factors and power distribution from the reference MCNP at three temperatures (800K, 1000K and 1200K) was the minimum.
11.1.4 Spectral Zones Optimization Methodology

The methodology for optimizing the spectral boundaries presented in this dissertation is based on the principle of preservation of reaction rates and currents in each zone. This was achieved by comparing the few-group NEM diffusion solution with the continuous-energy MCNP transport reference solution. The technique minimized the error between the two solutions by optimally repositioning the zone boundaries. The objective function for the optimization algorithm was defined as the sum of the fission, absorption and leakage rates error between MCNP and NEM.

The methodology required that the spectral effects of the adjacent zones be properly modeled. This was achieved by defining an iterative loop for optimizing the group-dependent bucklings. With the initial estimate of the group bucklings in MICROX-2, the diffusion constants are generated and supplied to NEM. Based on the output from NEM the partial currents are converted to groupwise net leakage terms, which are used together with the fluxes, diffusion coefficients and zone volumes to calculate new groupwise bucklings. The new buckling values are supplied to MICROX-2 and new average diffusion constants are generated. The updated cross sections are passed to NEM, and new fluxes and partial currents are determined. The process is repeated until the convergence criterion is met. This has proved to be an essential step in calculating accurate zone net leakages and accounting for spectral effects of the adjacent zones.

The optimization algorithm developed during this research identified optimum spectral boundaries based on the 5-zone, 6-zone and 7-zone core each at three temperatures. Significant improvement in the reaction rate errors were presented, with the
biggest improvement obtained with the 5-zone core. The basis for this observation is that the diffusion algorithms yield improved solutions with additional zones (mesh refinement); thus the additional zones in the 6-zone and 7-zone models would yield a solution closer to the reference solution based on the increased number of zones, and therefore a perceived smaller improvement in the error.

11.1.5 The Temperature Effect on Spectral Boundaries

Spectral zones were initially determined based on three temperatures which cover the range of the average fuel temperature at normal operating conditions: 800K, 1000K, and 1200K. The models assumed uniform temperature in the core and reflectors. The optimization methodology identified spectral zones that are consistent for the 3 temperature cases. The identified spectral boundaries at these temperatures agreed to ±2cm based on the 8-group structure. It is expected that with further increase of the number of energy groups towards spectral converged solutions the spectral boundaries for different temperatures will be the same. The obtained results demonstrated that the selected 8-group model provides predictions very close to such spectral converged solutions.

A realistic temperature profile was also applied to the core model and the spectral boundaries showed a minimal change when compared with the uniform temperature models.
It is therefore concluded that the temperature has minimal effect on the identification of optimum spectral boundaries when an appropriate few-group energy structure is selected to provide spectral converged solutions.

11.1.6 Identification of Spectral Boundaries Using Spectral Indices

The optimization methodology for identifying spectral zones is not necessarily a fast method since it involves several iterative loops. A practical spectral index has been defined in this dissertation that identifies spectral boundaries for the PBR core using diffusion-only data. The spectral index of group surface currents-to-group surface fluxes, and the spectral index of group surface currents-to-total surface fluxes revealed a series of minima and maxima points along the axial and radial dimension of the core. These minima and maxima points were found to correspond to the identified spectral boundaries based on the optimization algorithm. This approach proved to be consistent in identifying spectral boundaries with acceptable accuracy for the 8-group and 13-group structures. The best spectral boundaries for both the homogenized and heterogeneous cores were found to be comparable based on both group structures, with small differences due to the spectral shifts introduced by varying the material number densities in the heterogeneous core model.

The spectral index approach does not eliminate the need to use the optimization algorithm with the reference transport solution. In fact the optimization approach is still a very good and recommended approach since it will identify the optimum boundaries even if fewer than needed zones are specified in the problem. This was observed with the
results of the homogeneous case where 4 optimally positioned spectral boundaries yielded significant improvements to the results of a 5-zone core.

### 11.1.7 Optimum Spectral Boundaries

Radial spectral zones in the core were found to be the most important in analyzing the PBMR core. This importance is based on the heterogeneity of the core/reflectors configuration in the radial dimension, where the effect of the geometry and dimensions of the core and reflectors all had significant impact on the neutronics of this core.

In the axial dimension, the position of maximum power density was identified as a spectral boundary for all of the investigated core configurations. However, based on the approach of re-circulating the fuel in the core, the burnup variation in the axial dimension is significant. To properly account for the varying burnup, homogeneous material regions several centimeters in length are created to represent the axial burnup distribution for the equilibrium core. Since few group diffusion data has to be supplied for each material zone, defining spectral zones did not have a huge impact on the analysis. The mesh size within these material regions depend on the diffusion code used and on obtaining spatial convergence of the model. It was established that an axial mesh structure of 25cm would yield accurate results for a burnup mesh of 50cm.

The top and bottom reflectors only required 3 spectral zones, with the two small spectral zones of 10 to 15cm located close to the core/reflectors interfaces. In the side reflector, two spectral zones were also established, with the first zone having a dimension of 12cm. It was sufficient to define the rest of the side reflector up to the core barrel, as
one spectral zone. In the central reflector, 4 spectral zones were identified, with the first three zones located close to the core/reflectors interface. It was expected to have more zones in the central reflector compared to the other reflectors because of its neutronic importance. Fast neutrons leak out of the core and thermal neutrons are reflected back into the core with the higher probability of causing fission.

An important note on the reflectors is that the definition of the mesh in all reflectors is very important for the diffusion code to yield accurate results. Improperly defined mesh sizes in the reflectors were found to yield negative fluxes with the NEM code. Thus, the defined reflector spectral zones above do not eliminate the need for proper definition of nodes dimensions in the reflectors. It is recommended to always verify spatial convergence of the diffusion solution.

In summary, a spectral zones optimization methodology has been developed. Reactor core analyses based on the identified spectral zones have been shown to yield results that are closer to the transport reference MCNP solution without a significant increase of computational effort. The adequacy of the NEM code to analyze the PBR core using optimum input parameters has been presented. The 5-, 6- and 7-zone core models all yield excellent agreement of the power distribution when compared to the MCNP reference solution. The small differences in the $k_{\text{eff}}$ for the different zone models can be corrected by implementing a correction factor similar to discontinuity factor in LWR analysis to improve the flux distribution predictions at the core/reflectors interfaces.
11.2 Recommendations for Future Work

The following are recommended as future activities relating to this research.

11.2.1 The Heterogeneous Fuel Model

The optimization methodology that has been developed for the determination of spectral zones was based on a homogenized fuel model. It was pointed out that the effective multiplication factor based on the homogeneous case is underestimated. Therefore a heterogeneous fuel model is expected to have a neutron spectrum that is somewhat different from the one of homogenized fuel model. It would therefore be necessary to verify the results developed in this dissertation with the results of a heterogeneous fuel model. The heterogeneous fuel simulation will impact both Monte Carlo modeling and MICROX-2 modeling.

11.2.2 Optimum Energy Group Structure

The need for a proper energy group structure to analyze the PBR core has been identified in this dissertation. The need is based on the characteristics of graphite as a moderator. The group structure identified in this dissertation is not presented as the optimum group structure, but rather as the best one to use for this research based on available structures. This structure was optimized to yield excellent results in this research. It is however recognized that a methodology may need to be developed to
identify the optimum group structure for PBR core analyses. There are plans underway at Penn State in co-operation with INL to take this investigation forward.

Reviewing the figures showing the spectral ratio of surface currents to surface fluxes presented in this dissertation for both homogeneous and heterogeneous core models, groups 2 and 3 consistently identified the same spectral boundary. This may indicate that combining these 2 groups to form a seven-group structure may result in a group structure that is as good as the 8-group structure. This option should be explored in the future.

11.2.3 Spectral Zones for the Startup Core

The PBMR400 models analyzed in this dissertation were all based on the equilibrium fuel. Since it takes several cycles to achieve equilibrium core conditions, it would be useful to check the spectral zones developed in this dissertation with core models that are not at equilibrium, and for startup core with different uranium enrichment. It may also be of interest to the reactor physicists to verify these spectral zones based on equilibrium fuel at cold conditions following a shutdown.

11.2.4 Temperature Profile in the Reflectors

In this dissertation, the temperature effect on the spectral zones was investigated using uniform temperature models and a model with an exact fuel temperature profile. In all cases investigated, the reflectors were all at uniform temperature. It has been shown
that the moderator temperature has an effect on upscattering in the thermal energy range, particularly in the region of low-lying plutonium resonances. An investigation of spectral zones in the reflectors based on the more realistic temperature profile may be a useful case to investigate to verify the spectral zones identified in this dissertation.

### 11.2.5 Transport Correction Factor

In comparisons of the NEM and MCNP fluxes it was identified that diffusion theory incurs errors in analysis at boundaries between medium of high and low absorptions. Thus the neutron flux near the reflector/core interfaces will exhibit differences from the MCNP reference fluxes. In addition, the $k_{\text{eff}}$ will always be higher than the reference solution’s $k_{\text{eff}}$, because of diffusion theory’s larger extrapolation lengths at the two reflectors. A transport theory correction factor similar to discontinuity factor in LWR analysis has to be applied at the core/reflectors interfaces if the flux calculations are to be correct. This can be done using modern equivalence theory.

### 11.2.6 Practical Implementation Challenges

In this work the homogenized material definitions and distributions were used. As explained in Chapter 3.2 several so-called batched of fuel are mixed together in a given volume as fuel is re-circulated in the core, with the burnup and isotopic compositions of each batch traced individually. A further complication is also introduced by the pebble flow lines through the core where fuel spheres move at different speeds depending on
their proximity to the reflector boundaries and relative azimuthal positions relative to the
de-fuel chutes. In defining the optimum spectral zones as defined in this work these
variations (batches, flow-lines) needs to be incorporated. In principle this is straight
forward but the practical implementation will require delicate data manipulation to
correctly mix the different batches to obtain the representative fuel mixture in the spectral
zone, and afterwards to again obtain the representative microscopic cross sections for
each batch to perform batch power and depletion calculations.
Bibliography


35. Walsh GR, Methods of Optimization, 1975.


## Appendix A

General Atomics 193-Fine Group Structure

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# Appendix B

## A List of Nuclides in the PBMR400 Model

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3. **Other Nuclides**

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Appendix C

MCNP Homogeneous Core Axial Results

The MCNP homogeneous core axial reference results are presented in Figures C.1 to C.3.
Figure C.2: MCNP Homogeneous Core Axial Fission Rate (1000K)

Figure C.3: MCNP Homogeneous Core Axial Power Density (1000K)
Appendix D

MCNP Heterogeneous Core Axial Results

The MCNP heterogeneous core axial reference results are presented in Figures D.1 to D.4.
Figure D.2: MCNP Heterogeneous Core Axial Fission Rate (1000K)

Figure D.3: MCNP Heterogeneous Core Axial Power Density (1000K)
Figure D.4: MCNP Heterogeneous Core Axial Leakage Rate (1000K)
Appendix E

MCNP Heterogeneous Core with Temperature Profile Axial Results

The MCNP axial reference results of the heterogeneous core model with the actual temperature profile are presented in Figures E.1 to Figure E.4.

Figure E.1: MCNP Heterogeneous Temperature Model Axial Absorption Rate
Figure E.2: MCNP Heterogeneous Temperature Model Axial Fission Rate

Figure E.3: MCNP Heterogeneous Temperature Model Axial Power Density
Figure E.4: MCNP Heterogeneous Temperature Model Axial Leakage Rate
Appendix F

Spectral Ratio of Net Surface Current to Surface Fluxes Based on 13 Groups

The plots of the spectral index of net surface currents to surface fluxes for the homogeneous PBMR400 core in 13 energy groups are plotted in Figures F.1, F.2, F.3 and F.4. In Table F.1 the spectral boundaries identified from these figures are compared to the 8-group spectral boundaries presented in Chapter 7 (in Table 7.2).

Figure F.1: Net Surface Current-to-Surface Flux: Group
Figure F.2: Net Surface Current-to-Surface Flux: Groups 3, 4, 5 and 6
Figure F.3: Net Surface Current-to-Surface Flux: Groups 7, 8 and 9
Figure F.4: Net Surface Current-to-Surface Flux: Groups 10, 11, 12 and 13

Table F.1: Comparison of Spectral Index Boundaries

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VITA

Ramatsemela Mphahlele

Education

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1996  Baccalaureus Technologiae: Chemical Engineering
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2008  Doctor of Philosophy: Nuclear Engineering
      The Pennsylvania State University, Pennsylvania, USA

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1999  - 2005:  National Nuclear Regulator, Centurion, South Africa
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               •  Radiochemist – environmental verification program for
                  nuclear licence holders

1995  - 1999:  Koeberg Nuclear Power Station, Duynefontein, South Africa
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               •  Shift Chemist (plant operations)
               •  Technician - operator (water production plant)
               •  Trainee – comprehensive training in the Chemistry Department