The impact of homogenized cross-section correction mechanisms in OSCAR-4 as applied to SAFARI-1 research reactor

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Abstract

The nodal solver OSCAR-4 reactor analysis system contains a series of approximations (non-linear extensions) which aim to correct the full-core nodal calculation (mostly via corrections to the homogenised cross-sections) for typical errors induced during coarse-mesh homogenisation and group condensation. These schemes are intended to correct the nodal diffusion result as compared to an idealised full-core transport solution, which is in practice seldom performed or even practical to attempt. These schemes were developed for PWRs and the application and relevance of these schemes to highly heterogeneous research reactor designs have not as yet been fully quantified. This work focuses on the analysis of the cross-section re-homogenisation correction scheme. The purpose of this work is to perform an evaluation of this non-linear model as implemented in OSCAR-4, specifically with respect to the newly proposed OSCAR-4 SAFARI-1 core model. The new model is based in part on nodal cross-sections generated from the Monte Carlo based Serpent code. Serpent is a consistent reference transport solution against which the capability of the re-homogenisation scheme is measured. The SAFARI-1 mini-core model results show that the scheme is applicable in some cases, like the fuel-follower. In the full-core model, the environmental error due to infinite lattice approximation was 252 pcm, 2.30 % in average assembly power and 4.59 % in maximum power. The scheme reduced these to 88 pcm, 1.69 % and 3.52 % respectively. The scheme should therefore be applied selectively in the full-core to maximise its capability. The work will support both the verification and validation of SAFARI-1 reactor models.

Keywords: Nodal diffusion methods; spatial homogenisation; re-homogenisation; infinite fuel lattice; equivalence theory; environmental error; cross-section moments; form functions.
List of Abbreviations

This is a list of abbreviations used in this dissertation listed in alphabetical order

ANM  Analytic Nodal Method
ARI  All Rods In
ARO  All Rods Out
BA   Burnable Absorbers
BA/F-W Fuel assembly with burnable absorbers, placed next to a water-box
BOC  Beginning Of Cycle
BTE  Boltzmann Transport Equation
CORANA CORe ANAlysis
CROGEN CRoss-section GENeration
F-FF  Fuel assembly placed next to a fuel-follower
F-W  Fuel assembly placed next to a water-box
FF-W  Fuel-follower placed next to a water-box
HEADE HEterogeneous Assembly DEpletion
HEU  Highly Enriched Uranium
LEU  Low Enriched Uranium
JEFF Joint Evaluated Fission and Fusion
LINX Cross-section library linking code
LWR  Light Water Reactor
MANM Multi-group Analytic Nodal Method
MC  Monte-Carlo
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<td>MGRAC</td>
<td>Multi-Group Reactor Analysis Code</td>
</tr>
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<td>MTR</td>
<td>Material Testing Reactor</td>
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<tr>
<td>MW</td>
<td>Mega Watts</td>
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<td>Necsa</td>
<td>South African Nuclear Energy Corporation</td>
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<td>NEM</td>
<td>Nodal Expansion Method</td>
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<td>NTE</td>
<td>Neutron Transport Equation</td>
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<tr>
<td>OSCAR-4</td>
<td>Overall System for the CAIculation of Reactors version 4</td>
</tr>
<tr>
<td>POLX</td>
<td>Polynomial cross-section fitting code</td>
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<tr>
<td>PWR</td>
<td>Pressurised Water Reactor</td>
</tr>
<tr>
<td>RRA</td>
<td>Radiation and Reactor Analysis</td>
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<td>RRT</td>
<td>Radiation and Reactor Theory</td>
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<tr>
<td>RS</td>
<td>Radiation Science</td>
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<td>R&amp;TD</td>
<td>Research and Technology Development</td>
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<tr>
<td>SAFARI–1</td>
<td>South African Fundamental Atomic Research Installion 1</td>
</tr>
<tr>
<td>SOC</td>
<td>State Owned Company</td>
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<tr>
<td>WIMS</td>
<td>Winfrith Improved Multi-group Scheme-D</td>
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Chapter 1

Introduction

1.1 Background

A nuclear reactor core can generally be described as a complicated collection of components called assemblies, made up of an ensemble of different materials that maintain fission chain reactions, producing a steady population of neutrons. Neutrons interact with heavy fissile nuclei (such as uranium), which fission (split), releasing energy and more neutrons. The released neutrons interact with more nuclei causing more fissions, perpetuating the fission chain reaction (Duderstadt and Hamilton [1976]). Various assembly types, including fuel, control and reflector assemblies are arranged in some way to make up the reactor core. These fission reactions occur in the reactor core.

It is essential to the reactor analyst to have knowledge of quantities which influence the reactor operation. These quantities include power distributions, shut-down margins, isotopic depletion rates as well as many other reactor parameters. A number of reactor analysis procedures and computer codes have been developed to model the reactor core such that these parameters are determined as accurately and as fast as possible.

Reactor analysis applications include, but are not limited to, steady state neutron flux distribution calculations (to determine neutron flux and power distribution throughout the
reactor core as a function of energy and position), core-follow calculations (analysis focused on modelling material transmutation through the reactor cycle, comprised of a combination of flux and depletion calculations) and core reload analysis (a series of steady state core calculations to confirm that the fuel loading and core configuration for an up-coming cycle is within operating technical specifications).

The central problem in the applications listed above and other reactor analysis applications, lies within the ability to accurately predict neutron distribution in space, velocity and time. The neutron distribution can be determined by solving the neutron transport equation on the scale of the reactor core. Solving the neutron transport equation is a complex process even for modern, fast, multi-core computers. For practical solutions and for this idealised equation to be tenable, some approximations are applied.

The complexity of the nuclear reactor core makes it computationally impossible to directly solve the neutron transport equation analytically, especially for the full-core. Some modern reactor analysis procedures use the so called “deterministic” calculation path.

The deterministic reactor calculation path, often based on nodal diffusion theory, follows a two stage approach to simulating reactor cores (Duerigen 2013). The first stage is the homogenisation of cross-sections on the assembly level, to produce spatially homogenised and energy condensed assembly cross-sections for each reactor component. Homogenisation is achieved through 2D transport calculations, usually referred to as lattice calculations. The aim of homogenisation is to reduce the complexity of the problem, by averaging the assembly cross-sections, while preserving integral quantities of the transport calculation. In the second stage, the produced homogenised cross-sections are used in a diffusion calculation. The 2D homogenised regions are stacked together, axially, to simulate the 3D full reactor core, such that the required parameters like the k-eff, flux and power distribution can be determined.

Fuel assemblies are usually shuffled around the core from cycle to cycle. This means that a single fuel assembly goes into many different positions in it’s life time in the core. It is impossible to model and prepare appropriate cross section for all the numerous possible environments that the fuel assemblies can pass through when doing the lattice calculations.
Approximate boundary conditions are therefore used in the lattice calculations. The real core environment however, can be significantly different from the approximate environment used in the lattice calculation, giving rise to the concept of the environmental error. According to Smith et al. (1992) the environmental errors account for not more than 2% in power reactors. The term error in this context refers to the difference between reactor parameters calculated using a nodal method compared to those calculated using high-order (detailed) Monte Carlo transport method, sometimes referred to as the reference solution. In this work, we will consider these errors in the Material Testing Reactor (MTR) context, particularly SAFARI-1. MTRs are often referred to as research reactors as well.

Some schemes have been developed to mitigate against these environmental errors when performing reactor calculations. One such scheme is called the spatial re-homogenisation cross section correction scheme. The scheme was developed following the work done by Smith and Koebke (Smith, 1994; Koebke et al., 1985). It reduces the environmental error in the reactor calculations through cross section correction factors determined in the lattice calculation. Flux shape data from the lattice calculation is used to modulate the homogeneous flux in the nodal calculation. This improves the assembly flux from the approximate flux used in the lattice calculation. The improved flux is used to recompute homogenised cross-sections and therefore improves the nodal solution by the superposition of the average flux with the localised flux shape.

The re-homogenisation scheme was developed for Light Water Reactor (LWR) applications although it has been adapted for use in research reactor simulations as well. Research reactors, due to their very heterogeneous nature, are prone to substantial environmental dependency of the homogenised neutron cross-sections. Traditionally, larger numerical uncertainties could be tolerated in research reactors due to very conservative safety margins as well as very little or no financial pressure. However, increased commercial applications have resulted in aggressive operating strategies as in the case of the SAFARI-1 reactor. As a result, more accurate calculations have become a priority. One of the major challenges in reactor analysis and certainly in the analysis of research reactors, is the reduction of the
environmental error.

SAFARI-1 is a 20 MW tank-in-pool type MTR, owned and operated by the South African Nuclear Energy Corporation SOC Ltd. (Necsa), located at its Pelindaba site near Pretoria. In this work, we analyse the re-homogenisation cross section correction mechanism as applied to the SAFARI-1 research reactor. The efficiency and accuracy improvement of the re-homogenisation scheme to the highly heterogeneous research reactor designs have not yet been formally investigated.

1.2 Aim

We aim to determine whether the re-homogenisation scheme, as applied in the SAFARI-1 research reactor, is able to mitigate the environmental error sufficiently for use in the more heterogeneous research reactor core designs.

We are mainly concerned with the application and accuracy of these approaches in the research reactor designs, particularly the SAFARI-1 research reactor. The insights gained in this work can be applied to other existing and new research reactor designs.

1.3 Objectives

The specific objectives of this project are as follows:

- To isolate and quantify typical environmental errors introduced in the modelling of the SAFARI-1 reactor with the current reactor analysis deterministic calculation path.
- To evaluate the capacity of the already implemented re-homogenisation scheme to correct the environmental errors.
- To possibly propose improvements to both the scheme itself and to an improvement in the application regime.
1.4 Dissertation Outline

This chapter briefly describes the deterministic calculation path as applied by deterministic reactor analysis codes like OSCAR-4. A brief outline of the source of errors encountered in the path is given. The problem statement and research objectives are outlined as well.

Chapter 2 gives a brief account of the development of reactor analysis methods. It then provides a detailed description of the transport and diffusion theory culminating to a description of the re-homogenisation correction mechanism.

Chapter 3 describes the computer codes and models used in this study. The OSCAR-4 code system, Serpent and the OSCAR-Serpent link are described. Various mini-core models and full-core models used to analyse the environmental error are also described.

Chapter 4 and Chapter 5 provide the results for the various mini-core and full-core calculations, respectively. The effect of re-homogenisation on the equivalent parameters for each of the models are analysed. The effectiveness of the re-homogenisation mechanism in the various models of the research reactor is evaluated.

Conclusions are drawn in Chapter 6. In this chapter we discuss the major findings on the suitability of the re-homogenisation scheme in the SAFARI-1 reactor as a way of improving reactor analysis results. We discuss SAFARI-1 configurations where the scheme works well and where it fails. We also provide the scope for the future work that may be explore to further improve the applicability of the scheme in research reactor designs.

1.5 Conclusions

It is essential for reactor analysts to accurately predict some important reaction operational and safety parameters. This is achieved by accurately determining the neutron distribution in the reactor core.

Numerous computer codes have been developed so as to carry out this task with relative
ease. Nevertheless, this is still a daunting task due to the complexity of the nuclear reactor. A two-stage deterministic calculational procedure is generally used for reactor analysis. The procedure starts with homogenisation of cross-sections followed by the diffusion calculation. Fuel assembly cross-sections are often homogenised in approximate environments due to mobility of fuel assemblies, giving rise to the environmental error.

The re-homogenisation scheme was developed to mitigate against the environmental error. The scheme is part of the deterministic reactor analysis path. The function of the scheme is to reduce the environmental error obtained when fuel cross-sections from an infinite environment are introduced during reactor calculations. The scheme was particularly developed for power reactor designs although its applications has been extended to research reactor designs. In this work, we investigate the ability of the scheme to reduce the environmental error, in the research reactor design space.

We now proceed to look at how the re-homogenisation scheme fits into the deterministic path.
Chapter 2

Theory

2.1 Introduction

Nuclear reactor analysis involves the use of computational methods for predicting the free neutron population as stated in Section 1.1. Most of the other parameters like power distribution, shut-down margin, excess reactivity and many other reactor operational and safety parameters can simply be derived from this neutron distribution, once it has been accurately determined. It is therefore necessary to accurately characterise the neutron distribution in the reactor core such that other required quantities can in-turn be determined. The neutron distribution is governed by a fairly established mathematical model called the Boltzmann Transport Equation (BTE) (Cai 2014). Neutron distribution is modelled using a linear version of the BTE known as the Neutron Transport Equation (NTE) (Cho 2012). Although the NTE is a simplified form of the BTE, to solve it can still be very involved.

Over many years, dating back to the 70s and 80s, a series of simplifications has been developed to allow for the simulation of a snapshot reactor core flux distribution in a matter of seconds and the simulation of a full reactor cycle in a matter of minutes on a desktop computer.

In this chapter we will mainly focus on the series of these simplifications, approximations
and calculations applied in day-to-day reactor analysis. These simplifications enable reactor analysis to be performed at a full core-level with fairly good accuracy and short calculation times. We will also look at the errors associated with these approximations and how these errors can be reduced. In particular we will analyse the source of the environmental error and test the application of cross-section re-homogenisation.

### 2.2 Neutron Transport Theory

The NTE is the most fundamental and exact description of the distribution of neutrons in space, energy, time and direction of motion in the reactor. It is usually the starting point even for approximate solution methods. The NTE is derived from a particle balance on a particular volume, making a few assumptions that do away with generally phenomena which are unimportant for reactor analysis, such as neutron-neutron interactions.

#### 2.2.1 The neutron transport equation

The time dependent NTE equation is given below (Sekimoto, 2007):

\[
\frac{1}{\nu} \frac{\partial \psi(\vec{r}, \vec{\Omega}, E, t)}{\partial t} + \vec{\Omega} \cdot \nabla \psi(\vec{r}, \vec{\Omega}, E, t) + \sigma_t(\vec{r}, E) \psi(\vec{r}, \vec{\Omega}, E, t) = \\
\int_{4\pi} \int_0^\infty \sigma_s(\vec{\Omega}' \rightarrow \vec{\Omega}, E' \rightarrow E) \psi(\vec{r}, \vec{\Omega}, E, t) d\vec{\Omega}' dE' + \\
\frac{\chi(E)}{4\pi} \int_{4\pi} \int_0^\infty \nu(E) \sigma_f(\vec{r}, E') \psi(\vec{r}, \vec{\Omega}', E', t) dE' d\vec{\Omega}'
\]  

(2.1)

where

- \( \psi(\vec{r}, \vec{\Omega}, E, t) \) = angular neutron flux as a function of space (\( \vec{r} \)), angle (\( \vec{\Omega} \)), energy (E) and time (t),
- \( \sigma_x \) = microscopic cross-section of type ‘x’ of which (t) is total, (f) fission and (s) scattering,
- \( \nu \) = average number of neutrons generated per fission, and
\( \chi(E)dE = \text{probability that a fission neutron is created in } dE \text{ about energy } E. \)

Equation 2.1 is derived based on mechanisms which are responsible for neutron production (right hand side) and neutron loss (left hand side).

Ideally, we would like to solve Equation 2.1 on the scale of the heterogeneous reactor core, in fine spatial, energy and angular detail. Considering that the equation has three spatial variables, two angular variables, one energy variable and time which ranges from milliseconds to years, solving this equation is a very expensive computational task.

In theory, the 3D neutron transport equation, (Equation 2.1) can be solved in the entire core, if thermal hydraulic properties and fundamental nuclear data of the reactor are available. A discretised three-dimensional, multi-group neutron transport equation can be solved using a fine mesh with uniform material properties within each such small region, obtaining multi-group flux solution for the whole reactor core, often referred to as the “heterogeneous” reference neutron transport solution (Forslund, 2000). However, due to the geometrical detail required to model the entire core, i.e. fuel plates, control rods, water gaps, including depletion regions (Smith, 1986), this is a time consuming process. It is therefore not feasible to solve the full core 3D transport equation directly within an acceptable time frame. The acceptable time frame in this context ranges from a few minutes to a few hours.

A well established and ever growing set of direct solution schemes for this equation exists. For some reactor physics applications, these direct solution schemes are practical and are applied on the scale of the full detailed reactor description. These schemes are becoming increasingly more viable with the continual development of computing technology, as financial costs continue to decline. For instance, a single point-in-time transport solution of the a PWR reactor core on a small cluster (say 10 to 20 computing cores) currently requires a calculational time in the order of hours to days.

However, complimentary to these highly accurate solution schemes, more efficient solution schemes are often required, where a large number of reactor core simulations are needed in
a relatively short time. These applications employ a number of simplifications, but allow for
the simulation of a relatively accurate solution, at assembly level, in a matter of seconds,
and the simulation of a full reactor cycle in a matter of minutes on a desktop computer.
In order to achieve this kind of benefit at an acceptable accuracy, a multi-step approach to
solving Equation 2.1 is employed. Notwithstanding the considerable advances in computer
technology, few group nodal diffusion theory methods still prevail in global reactor analysis
(Müller 1989).

For most routine reactor calculations, the steady state conditions are sufficient, hence the
time independent neutron transport equation (Eq. 2.2 below) is often used (Stacey 2007):
\[
\bar{\Omega} \cdot \nabla \psi(\vec{r}, \bar{\Omega}, E) + \sigma_t(\vec{r}, E)\psi(\vec{r}, \bar{\Omega}, E) = 
\int_{4\pi} \int_{0}^{\infty} \sigma_s(\bar{\Omega}' \rightarrow \bar{\Omega}, E' \rightarrow E)\psi(\vec{r}, \bar{\Omega}, E)d\bar{\Omega}'dE' +
\frac{\chi(E)}{4\pi k} \int_{4\pi} \int_{0}^{\infty} \nu(E)\sigma_f(\vec{r}, E')\psi(\vec{r}, \bar{\Omega}', E')dE'd\bar{\Omega}' \quad (2.2)
\]
where

\[ k = k\text{-eigenvalue (multiplication factor) of the system.} \]

The k-eigenvalue modifies the number of neutrons produced by each fission to preserve the
global balance of neutrons. The ratio of the net loss-to-gain of neutrons is the k-eff. For a
reactor that is operating at a critical state, the value of k-eff is unity (i.e. k-eff = 1).

### 2.3 The Reactor Calculational Path

Solutions to Equation 2.2 can be divided into two broad categories namely Monte-Carlo and
deterministic methods. Monte-Carlo methods are sometimes referred to as probabilistic or
stochastic methods.


\section*{Chapter 2. Theory}

\subsection*{2.3.1 Monte-Carlo methods}

Monte-Carlo (MC) methods are used to simulate the physical processes that the neutron undergoes, without directly solving the neutron transport equation. These methods simulate the particle behaviour through a random walk process and use random numbers to record some aspects of the particle’s behaviour. The only requirement for these calculations is that the probability distribution functions for all the possible particle interactions, also called reactions, is known. Once these have been specified, the calculations proceed by the random sampling of the probability distribution functions. These high fidelity methods have the ability to represent complex geometries in multi-dimensional space, without numerous assumptions, usually implemented in 3D deterministic procedures. MC methods thus do not have discretisation errors but instead have statistical errors. The Monte carlo method treats all of space, energy and angle continuously.

The major advantages of the MC methods over the deterministic methods are the continuous energy treatment and the precise modelling that can be carried out on the 3D geometry, hence allowing for modelling freedom and access to very accurate fine scale flux profiles. While MC calculations produce very accurate results in complex geometries, their turnaround times are very long, to the extent that they are quite prohibitive for day-to-day support to reactor operations. In general MC, methods are currently being used for model and code verification purposes and not for routine calculations. Simulation of day-to-day operations is done via the deterministic calculation path.

\subsection*{2.3.2 Deterministic methods}

Deterministic methods use several approximations and discretisation of the independent variables e.g. space, energy and direction, together with the application of some numerical methods to solve the NTE. The solution gives some information about the average particle behaviour. Independent variables (space, energy and direction) are transformed from continuous to a discrete representation. One or more numerical methods are used to solve the
NTE for overall particle behaviour. In the end, the transport problem is reduced to a set of linear equations that can be solved on a computer (Mervin 2013; Karriem 2012).

2.3.3 Assumptions and simplifications

The standard deterministic calculational approach employs a number of assumptions (Trkov and Ravnik 1994) in the modelling of the physical phenomena present in the operation of a reactor as follows:

1. Firstly, in thermal reactor designs, neutrons cause fission in the thermal range (in the order of eV), yet they are born in the fast range (MeV). They are moderated with relatively large energy losses per collision between these two energy ranges. Thus, the resolution of the energy variable could be simplified through the introduction of broad energy groups. A full-core solution with 2 to 10 energy groups would be capable of deducing the primary physical phenomenon. This is called energy group condensation, and requires that the condensed cross-section over the broad energy groups retain reaction rates deduced from the original fine-groups.

2. Secondly, for typical deterministic reactor analysis applications, it is of primary interest to determine the solution to the most important physical observables, such as reaction rates and power. For such applications, the detailed knowledge of the direction of travel of the neutron is not very important. Therefore, the solution scheme need only provide scalar flux as primary unknown as opposed to the angular flux.

3. Thirdly, it is observed that the fission process is the dominant reaction in a nuclear reactor core. The fission reaction is an isotropic event. This observation implies that the angular variable is not dominant and can potentially be treated in an approximate sense, on the scale of at least an assembly level. This allows for the possibility of applying some angular simplification to the transport equation, such as diffusion theory.

4. Lastly, for many analysis applications, a knowledge of region averaged (as opposed to fine minute detail) fluxes and reaction rates could be sufficient. This naturally leads to a
simplification of the spatial domain and the introduction of the homogenisation process to produce cross-section data on a simplified mesh. The requirement is that such homogenised, region-averaged, cross-sections retain the reaction rate of the original heterogeneous region.

We now consider each assumption in turn, to understand how each helps in simplifying the determination on neutron flux distribution.

2.3.4 Multi-group formulation

Considering Assumption 1 in Section 2.3.3, we note that the NTE is of continuous form in the independent variables. We therefore start off by discretising the energy variable in the equation into $G$ energy intervals. Integrating Equation (2.2) over energy group $g$, we can write the transport equation in its multi-group representation as (Duderstadt and Hamilton, 1976)

$$
\vec{\Omega} \cdot \nabla \psi^g(\vec{r}, \vec{\Omega}) + \sigma^g_t(\vec{r})\psi^g(\vec{r}, \vec{\Omega}) = \sum_{g'=1}^{G} \int_{4\pi} d^2 \vec{\Omega}' \sigma^g_{s}(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega})\psi^{g'}(\vec{r}, \vec{\Omega}') + \frac{1}{4\pi} \chi^g \sum_{g'=1}^{G} \nu \sigma^g_{f}(\vec{r})\psi^{g'}(\vec{r}) + S^g(\vec{r}, \vec{\Omega})
$$

(2.3)

where $g=1, G$.

Assuming energy separability in each energy group, we have

$$
\psi(\vec{r}, E, \vec{\Omega}) \approx f(E)\psi^g(\vec{r}, \vec{\Omega}), \quad E_g \leq E \leq E_{g-1}
$$

(2.4)

where $f(E)$, is the energy dependent shape function such that

$$
\int_g dE f(E) = 1.
$$

(2.5)

The group angular flux is defined as:

$$
\psi^g(\vec{r}, \vec{\Omega}) = \int_g dE \psi(\vec{r}, E, \vec{\Omega}).
$$

(2.6)
Multi-group parameters are then defined as follows:

\[ \sigma_g^t(\vec{r}) = \int_g dE\sigma_t(\vec{r}, E) f(E), \]  
\[ (2.7) \]

\[ \nu\sigma_g^f(\vec{r}) = \int_g dE\nu\sigma_t(\vec{r}, E) f(E), \]  
\[ (2.8) \]

\[ \sigma_{s}^{g'\rightarrow g}(\vec{r}, \vec{\Omega} \rightarrow \vec{\Omega'}) = \int_g dE \int_{g'} dE' \sigma_s(\vec{r}, E' \rightarrow E, \vec{\Omega'}), \]  
\[ (2.9) \]

\[ \chi^g = \int_g dE\chi(E), \]  
\[ (2.10) \]

\[ S_g(\vec{r}, \vec{\Omega}) = \int_g dE S_g(\vec{r}, E, \vec{\Omega}). \]  
\[ (2.11) \]

### 2.3.5 Multi-group diffusion representation

Considering Assumption 2 in Section 2.3.3, we integrate Equation 2.3 over all angles to obtain the multi-group balance equation (Bell and Glasstone [1970]),

\[ \vec{\nabla} \cdot \vec{J}_g(\vec{r}) + \sigma_g^t(\vec{r})\phi_g(\vec{r}) = \sum_{g' = 1}^G \sigma_{s}^{g'\rightarrow g}(\vec{r})\phi_{g'}(\vec{r}) + \chi^g \sum_{g' = 1}^G \nu\sigma_g^f(\vec{r})\phi_{g'}(\vec{r}) + S_g(\vec{r}), \]  
\[ (2.12) \]

with group current defined as:

\[ \vec{J}_g(\vec{r}) = \int_{4\pi} d\Omega\vec{\Omega}\psi_g(\vec{r}, \vec{\Omega}). \]  
\[ (2.13) \]

The group scalar flux is given by:

\[ \phi^g(\vec{r}) = \int_{4\pi} d\Omega\psi^g(\vec{r}, \vec{\Omega}), \]  
\[ (2.14) \]

the group external source as

\[ S^g(\vec{r}) = \int_{4\pi} d\Omega S^g(\vec{r}, \vec{\Omega}), \]  
\[ (2.15) \]

and the group-to-group scattering cross-section as

\[ \sigma_{s}^{g'\rightarrow g}(\vec{r}) = \int_{4\pi} d\Omega\sigma_{s}^{g'\rightarrow g}(\vec{r}, \vec{\Omega'} \rightarrow \vec{\Omega}). \]  
\[ (2.16) \]
The problem with Equation 2.12 is that both the scalar flux and current are unknown and there is no direct way of relating to them. From Assumption 3 in Section 2.3.3, we can introduce diffusion theory as an alternative to transport. This approximation is valid if the angular flux is only linearly anisotropic. This means that neutron interactions with matter exhibit only weak angular dependence.

Diffusion theory is introduced by assuming that neutrons obey Fick’s Law, which is stated as (Stacey, 2007)

\[
\vec{J}^g(\vec{r}) = -D^g(\vec{r}) \nabla \phi^g(\vec{r}).
\]  (2.17)

Introducing this relationship between scalar flux and current, we obtain the multi-group diffusion equation

\[
-\nabla \cdot D^g(\vec{r}) \nabla \phi^g(\vec{r}) + \sigma_t^g(\vec{r}) \phi^g(\vec{r}) = \sum_{g'=1}^{G} \sigma_{s0}^{g'\rightarrow g}(\vec{r}) \phi^{g'}(\vec{r}) + \chi^g \sum_{g'=1}^{G} \nu \sigma_{f}^{g'}(\vec{r}) \phi^{g'}(\vec{r}) + S^g(\vec{r}).
\]  (2.18)

Equation 2.18 shows a simplified energy representation, angular representation and defines the primary unknown as the scalar flux. However, the spatial variable needs to be simplified as well, for a significantly fast solution. It is important to note at this stage that the solution is usually sought on large homogeneous zones called nodes, rather than on a fine mesh.

### 2.3.6 Nodal diffusion

From Assumption 4, we consider that the solution is not sought on a fine mesh but on large homogeneous regions called nodes. A node can be to the order of a fuel assembly or more in the two radial dimensions and more or less the same size axially. Homogenisation is performed at this nodal level.

Making the assumption that the solution is sought in one node and that the material properties for the node are provided, we can cast Equation 2.18 into a 3D nodal diffusion equation.

\[
-D_n^g \nabla^2 \phi_n^g(u, v, w) + \sigma_n^{g,\text{rem}} \phi_n^g(u, v, w) - S_n^g(u, v, w) = 0.
\]  (2.19)
Note also in the equation that the radial dimension is split into 3 explicit coordinate directions \((u, v, w)\). The within group scattering cross-section is subtracted from the total cross-section to obtain the removal cross-section.

Equation 2.19 is obtained by dividing space into \(n\) nodes with node \(n\) having sizes \((h_{n,u}, h_{n,v}, h_{n,w})\). Integrating Equation 2.19 over the volume \(V_n\) then divided by the node volume and after applying the divergence theorem, we obtain the nodal balance equation,

\[
\sum_{m=1}^{6} a_{nm} \mathcal{J}_{mn}^g + \sigma_{n}^{g,\text{rem}} \overline{\phi}_n^g = \overline{S}_n^g, \tag{2.20}
\]

where

\[
\overline{\phi}_n^g = \frac{1}{V_n} \int_{V_n} \phi_n^g(u, v, w) dV_n, \tag{2.21}
\]

\[
\mathcal{J}_{mn}^g = -\frac{D_n^g}{s_{mn}} \frac{\partial}{\partial n} \int_{S_{mn}} \phi_n^g(u, v, w) dS_{mn}, \tag{2.22}
\]

and the node-averaged source in energy group

\[
\overline{S}_n^g = \frac{1}{V_n} \int_{V_n} Q_n^g(u, v, w) dV_n. \tag{2.23}
\]

In Equation 2.20, \(\mathcal{J}_{mn}^g\) denotes the normal component of the side-averaged net current on the surface between node \(n\) and \(m\) (with the normal pointing outward from node \(n\)), \(S_{mn}\) represents the surface between nodes \(m\) and \(n\). The term \(a_{nm}^{un}\) is the surface to volume ratio of that surface. The term, \(\overline{\phi}_n^g\) represents the node-averaged flux in energy group \(g\). The averaged flux on the interface between node \(n\) and node \(m\) will be denoted by \(\overline{\phi}_{mn}^g\).

The system however, is under-specified and various approaches are utilised within the class of nodal methods to find the relationship between the node-averaged fluxes and the side-averaged net currents, so that Equation 2.20 may be solved. This distinction in how the expression for side-averaged currents is obtained, is also the primary differentiating factor between the various classes of nodal methods. One such method is the transversely integrated nodal diffusion method.
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Transversely integration nodal diffusion methods

To obtain the average surface currents, $\mathcal{J}_{mn}^g$, most modern nodal codes utilise the transverse integration method (Prinsloo, 2012). Equation 2.18 is integrated across the area transverse to the direction of interest, to obtain 1D diffusion equations in each direction.

Starting from the time independent neutron transport equation (Equation 2.2), integrating the transport equation over all angles and applying Fick’s law, we have the diffusion equation in rectangular coordinates (Stacey, 2007),

$$-\nabla \cdot D_n^g(u,v,w) \nabla \phi_n^g(u,v,w) + \sigma_{t,n}^g(u,v,w) \phi_n^g(u,v,w) = Q_n^g(u,v,w),$$

(2.24)

where

$$Q_n^g(u,v,w) = \frac{1}{k_{\text{eff}}} \sum_{g' = 1}^G \chi^g \nu \sigma_{n,f}^{g'} \phi_n^{g'}(u,v,w) + \sum_{g' = 1}^G \sigma_n^{g'g'} \phi_n^{g'}(u,v,w),$$

(2.25)

expanding, we get

$$-\frac{\partial}{\partial u} D_n^g \frac{\partial}{\partial u} \phi_n^g(u,v,w) - \frac{\partial}{\partial v} D_n^g \frac{\partial}{\partial v} \phi_n^g(u,v,w) - \frac{\partial}{\partial w} D_n^g \frac{\partial}{\partial w} \phi_n^g(u,v,w) + \sigma_n^g \phi_n^g(u,v,w) = Q_n^g(u,v,w).$$

(2.26)

Integrating in the $v-$ and $w-$ direction to get the 1D diffusion equation in the $u-$ direction we have,

$$-\frac{\partial}{\partial u} D_n^g \frac{\partial}{\partial u} \phi_n^g(u) + \sigma_n^g \phi_n^g(u) = Q_n^g(u) - \frac{1}{h_{n,v}} L_n^g(u) - \frac{1}{h_{n,w}} L_n^g(u),$$

(2.27)

where

$$\phi_n^g(u) = \frac{1}{h_{n,v}} \frac{1}{h_{n,w}} \int dv \int dw \phi_n^g(u,v,w),$$

(2.28)
and

\[
L_{g,v}^n(u) = \frac{1}{\Delta w} \int dw [ -D_g \frac{\partial}{\partial u} \phi_n^g(u,v,w)]_{w^-}^{w^+}, \tag{2.29}
\]

\[
L_{g,w}^n(u) = \frac{1}{\Delta v} \int dv [ -D_g \frac{\partial}{\partial v} \phi_n^g(u,v,w)]_{v^-}^{v^+}. \tag{2.30}
\]

The 1D equation in the \( u \)– direction can be simplified to

\[
-D_n \frac{d^2}{du} \phi_n^g(u) + \sigma_{a,n}^{g,rem} \phi_n^g(u) = Q_n^g(u) - L_{g,vw}^n(u) \tag{2.31}
\]

where \( L_{g,vw}^n(u) \) is the transverse leakage term, \( \frac{1}{\Delta y} L_{g,v}^n(u) + \frac{1}{\Delta w} L_{g,w}^n(u) \).

The 1D equations in the \( v \)– and \( w \)– directions are derived in an analogous manner.

**Solutions to the 1D diffusion equations**

There are several variants of the transverse integrated nodal diffusion methods that have emerged; these can be distinguished by the methods used for solving the one dimensional diffusion equations [Lewins et al., 2002].

To solve the transverse integrated equations, several approaches have been developed. Since only node average surface leakages are known from a nodal solution, the transverse leakage spatial dependence need to be estimated. This is usually done using the quadratic polynomial, preserving the node average surface leakages of the node in question and its adjacent nodes along the direction of interest. The solution of the 1D neutron diffusion equations can be accomplished analytically - the analytic nodal method (ANM) [Smith, 1979; Cacuci, 2010] or using spatial trial functions - nodal expansion method (NEM) [Koyama and Aoyama, 1989]. The solution of the coupled nodal balance and transverse integrated equations completes the nodal solution [Prinsloo and Tomašević, 2008].

Deterministic calculational tools have become a standard for in-core neutronic analysis, particularly for core reload and core-follow type analysis. Nodal diffusion based methods,
over viewed in Lawrence (1986), with the primary formulations as the Nodal Expansion Methods Finnemann and Wagner (1977) and the Analytic Nodal Method Smith (1979), have remained the typical workhorse for industry in performing such work, and have persisted as such mostly due to their efficiency. Furthermore, due to a series of particular extensions to their initial formulation, these methods are still in active use today Smith et al. (1992).

2.3.7 Homogenisation

The nodal diffusion parameters mentioned above are obtained from lattice calculations. These are detailed neutron transport calculations performed in fine energy groups to produce multi-group parameters for each component in the core. These lattice calculations are independently performed for each material region with representative boundary conditions. The parameters are cross-sections that are tabulated against relevant state parameters. These are once-off calculations resulting in a library of tabulated assembly-homogenised cross-sections.

The homogenisation process makes it difficult to preserve spatial quantities in the smaller nodes. The usual procedure is to preserve spatial integrals of the quantities of interest. The most important quantities to be preserved are the node-averaged reaction rates, surface-averaged group currents and the reactor eigenvalue (Stammler and Abbate, 1983).

In this work, we will denote the homogenised parameters with a $\hat{\cdot}$. For instance, the homogenised multi-group cross-section for a reaction of type $x$ is given by $\hat{\sigma}_{n}^g$.

Comparing the multi-group version of the heterogeneous transport problem and the analogous equation for the homogenised model (Stacey, 2007) we have:

$$\begin{align*}
-\nabla \cdot \vec{J}^g(\vec{r}) + \sigma_t^g(\vec{r})\phi^g(\vec{r}) &= \sum_{g'=1}^{G} \sigma_{s0}^{g'\rightarrow g}(\vec{r})\phi^{g'}(\vec{r}) + \frac{\chi^g}{k_{eff}} \sum_{g'=1}^{G} \nu \sigma_f^{g'}(\vec{r})\phi^{g'}(\vec{r}) + S^g(\vec{r}), \\
-\nabla \cdot \vec{J}^{g}(\vec{r}) + \hat{\sigma}_{n}^g(\vec{r})\hat{\phi}^g(\vec{r}) &= \sum_{g'=1}^{G} \hat{\sigma}_{s0}^{g'\rightarrow g}(\vec{r})\hat{\phi}^{g'}(\vec{r}) + \frac{\chi^g}{k_{eff}} \sum_{g'=1}^{G} \nu \hat{\sigma}_f^{g'}(\vec{r})\hat{\phi}^{g'}(\vec{r}) + \hat{S}^g(\vec{r}),
\end{align*}$$

(2.32)  (2.33)
where both equations are cast in their eigenvalue form, and with the neutron source term written out in full.

The solution for Equation 2.32 gives a more accurate representation of the neutron distribution, but is very expensive. On a full-core scale, we would therefore rather compute the flux through Equation 2.33, because its solution is more efficient. We assume here that with appropriate definition of the nodal parameters, the task is achievable. To ensure that the homogeneous nodal solution is equivalent to the heterogeneous solution, we select the terms that need to be preserved when performing the homogeneous calculation. Generally, the nodal scalar flux, reaction rates in all groups as well as leakage terms need to be conserved. It then follows that the k-eff is also conserved.

To conserve the volumetric reaction rates for node \( n \), we have to impose that, for reaction type \( x \)

\[
\int_{V_n} \hat{\sigma}_x^g(\vec{r}) \hat{\phi}^g(\vec{r}) d\vec{r} = \int_{V_n} \sigma_x^g(\vec{r}) \phi^g(\vec{r}) d\vec{r} \quad \text{and} \quad \int_{S_n} \nabla \cdot \hat{J}_x^g(\vec{r}) \cdot dS = \int_{S_n} \nabla \cdot J_x^g(\vec{r}) \cdot dS \quad (2.34)
\]

where \( V_n \) is the volume on the node \( n \), and \( S_n^i \) is the \( i \)th surface of node \( n \).

From Equation 2.34 and assuming that all homogenised parameters are spatially constant within each node as well as by applying the diffusion approximation (Equation 2.17), we have:

\[
\hat{\sigma}_x^g = \frac{\int_{V_n} \sigma_x^g(\vec{r}) \phi^g(\vec{r}) d\vec{r}}{\int_{V_n} \phi^g(\vec{r}) d\vec{r}} \quad \text{and} \quad \hat{D}_x^g = -\frac{\int_{S_n^i} \hat{J}_x^g(\vec{r}) \cdot dS}{\int_{S_n^i} \nabla \phi^g(\vec{r}) \cdot dS}. \quad (2.35)
\]

Equation 2.35 states that the heterogeneous cross-sections should be flux-volume weighted in order to yield the desired parameters. It should be noted however that the full-core heterogeneous reference flux \( \phi^g(\vec{r}) \) is unknown. To overcome this problem, a single fuel assembly or a number of fuel assemblies (referred to as a colourset) are modelled within reflective boundary conditions, thus simulating an infinite array of fuel. A transport calculation is performed,
replacing the full-core heterogeneous flux solution with the heterogeneous solutions from these smaller regions.

In Equation 2.35, the expression for diffusion coefficient should be valid on all the surfaces of the node. This is in opposition to applying flux and current continuity with neighbouring nodes on each surface. So, the flux continuity with neighbouring nodes is violated. To match leakage on each surface, additional degrees of freedom are needed to allow the simultaneous preservation of reaction rates and surface currents.

However, the solution to a global homogenised reactor problem does not really preserve any of the parameters in Equations 2.32 and 2.33. These assembly flux-weighted cross-sections preserve reaction rates of the infinite lattice. In a realistic reactor, having finite boundaries or multiple assembly types, these reaction rates are not preserved. In order to improve the accuracy of node-averaged reactor properties predicted through the homogenised parameters discussed in Section 2.3.7, more advanced homogenisation methods have been developed. Koebke (Smith, 1986) formulated a mathematical interface condition which allows exact preservation of both reaction rates and net currents from the heterogeneous reactor problems (Pekicen, 2011) referred to as the generalised equivalence theory.

2.4 Generalised Equivalence Theory

The generalised equivalence theory provide an extra degree of freedom to match the homogeneous solution to the heterogeneous assembly level solution. This degree of freedom is represented in the form of additional homogenisation parameters known as discontinuity factors, which account for the loss of spatial resolution at the interface between assemblies during homogenisation (Smith, 1979).

Discontinuity factors are ratios of the node surface averaged heterogeneous flux to the corresponding surface average homogeneous flux. Together with other nodal equivalent parameters, discontinuity factors preserve the node surface averaged net leakage from the
heterogeneous calculation (Lawrence 1986).

\[ f_{n}^{g} = \frac{\hat{\phi}_{n}^{g}}{\phi_{n}^{g}} \]  

(2.36)

where \( f_{n}^{g} \) is the side discontinuity factor. Side discontinuity factors as shown in Equation 2.36 specify the ratio of the surface flux as produced by the assembly-level (heterogeneous) calculation and the surface flux by the equivalent (homogeneous) calculation.

Discontinuity factors are supplied to the subsequent full-core nodal calculation in order to simultaneously preserve the node surface average flux and net leakages from the heterogeneous calculation. While the homogenised cross-sections set the equivalence between the homogeneous and heterogeneous configuration in terms of reaction rates, discontinuity factors set the equivalence in terms of neutron leakage through the node boundaries (Smith 1986).

2.4.1 Practical applications of the deterministic path

Figure 2.1 shows a practical deterministic calculational path. The path proceeds from left to right, where it starts with 2D single- or multi-assembly (colourset) transport calculations in fine energy groups all the way to the 3D full-core nodal diffusion calculations (Akhmouch and Guessous 2003). As the path proceeds from left to right, the problem size increases exponentially, while the spatial and energy detail diminishes as homogenisation takes place.

The process in practice is then as follows:

1. Perform a 2D transport (or lattice) calculation on the assembly level in a typical environment (often reflective boundary conditions) by solving Equation 2.2 in fine energy and spatial detail. Note down the heterogeneous side-fluxes on all surfaces of the node in each group \( g \). This will normally be done for a range of all the expected future states of the assembly, since this calculation is typically done once and the results are stored. This means that lattice calculations are performed for, amongst
2. Tabulate node-averaged homogenised cross-sections and other equivalent parameters calculated via Equation 2.34. Use the flux solution from Step 1 as weighting function in space and energy.

3. Perform a 2D single-node homogeneous diffusion calculation, solve Equation 2.35 using the cross-sections obtained in Step (2) and impose the side-averaged transport currents as boundary conditions on each surface. Note down the homogeneous diffusion side-fluxes on each surface in each group $g$.

4. Calculate discontinuity factors on each surface of each node and store them along with the cross-sections obtained in Step 2. Together this data now represents the set of nodal equivalence parameters. There are additional equivalence parameters, such as intra-assembly form factors used for fine-scale flux reconstruction inside the node, but these are not discussed here.

5. Perform the 3D full-core solution by solving Equation 2.33 on the full-core level, using discontinuous boundary conditions between nodes as per Equation 2.36.
2.4.2 Full-core calculations

In order to solve the global reactor problem, a neutron balance equation is used for each node. The nodal balance equation is obtained by integrating the diffusion equation (with node-wise constant coefficients) over the node volume. By solving the diffusion equation locally within each node and imposing a continuity condition of the heterogeneous flux and the net current over the node boundaries, an expression for the node surface-averaged homogeneous flux gradient (i.e. net neutron current) as a function of the neighbouring node average fluxes may be obtained and used for nodal coupling. Consequently, a coupled set of non-linear equations with coefficients that depend on the flux solution itself is derived for the global problem with node average fluxes as unknowns. Due to the non-linear character of these equations, standard numerical iteration techniques have to be employed in order to get the flux solution.

2.5 Environmental Effects

For full equivalence between heterogeneous transport and homogeneous nodal diffusion, the nodal cross-sections and discontinuity factors must be generated for the assembly of interest in its correct neighbouring environment.

Complications arise when the real assembly environment differ significantly from the idealised conditions assumed in the single-assembly lattice calculation used for generating spatially homogenised and energy collapsed nodal cross-section data. The difficulty with calculating lattice parameters using Equations 2.35 and 2.36 is that the homogeneous flux has a spatial shape and energy spectrum associated with the single assembly infinite medium problem described in Section 2.3.7. It therefore lacks the effects of spatial and spectral interactions with adjacent lattice cells of different types as obtained in the actual core environment. However, for assemblies at the centre of a relatively homogeneous reactor core (like in power reactors for instance, where the core consists mostly of fuel) the homogeneous flux obtained
is likely to be a very good approximation of the heterogeneous flux. For the assemblies near the edges of the core, or between assemblies with very different material properties, or in highly heterogeneous cores like research reactors, there will be significant flux gradients. In these cases the infinite lattice assumption exhibits significant errors, since it is a poor approximation of the core flux.

In essence, the flux distribution of the operating reactor core differs from the lattice calculation flux. By imposing reflective boundary conditions in the single assembly calculations, environmental effects due to interactions with neighbouring nodes, are not properly accounted for in the cross-section homogenisation procedure. As a result, homogenisation errors are induced in the flux-volume-weighted nodal equivalent parameters to be used in the homogeneous coarse-mesh, few group nodal calculations.

In order to account for these effects, the nodal cross-sections have to be adjusted in some way when solving the global problem. However, real equivalence is guaranteed only if the flux shape inside the assembly in the core is close to the infinite medium flux shape, computed in lattice calculations (Forslund, 2000). This realisation gave rise to the concept of re-homogenisation.

A re-homogenisation method was designed to adjust infinite environment cross-sections to the current global environment.

### 2.6 Re-Homogenisation Method

Given the environmental error discussed above, we now strive to formulate the re-homogenisation procedure, which will allow for the correction of nodal cross-sections based on the true environment that the assembly experiences in the nodal core calculation.

For a given node, spatial homogenised and energy collapsed cross-sections, to be used in the global environment, are computed in the lattice calculation with reflective boundary conditions. In the real assembly environment, it is assumed that the assembly heterogeneous
flux can be approximated by the product of the single assembly flux form function and the core nodal homogeneous (average) flux solution. The single assembly form function is defined as

$$\phi(\vec{r}) \approx F^0(r)\hat{\phi}(\vec{r}),$$

(2.37)

where

$\phi(\vec{r})$ is the heterogeneous flux obtained in the lattice calculation, and

$\hat{\phi}(\vec{r})$ is the intra-nodal homogeneous flux distribution which is assumed to be the same as the equivalent homogeneous flux distribution.

$F^0(\vec{r})$ is the heterogeneous flux form function. It is the shape function for the infinite system, which describes the local periodic behaviour of angular flux within the node (Trahan and Larsen, 2015).

Considering a 2D space with two coordinate directions $u$, $w$ and a unit single assembly of radial mesh sizes $h_u$ and $h_w$. The spatially smeared (homogeneous) node cross-sections in the Cartesian coordinate system is given by Equation 2.35. Neglecting the energy variable and writing out in 2D, we have,

$$\hat{\sigma} = \frac{\int_{h_u} du \int_{h_w} dw \sigma(u,w)\phi(u,w)}{\int_{h_u} du \int_{h_w} dw \phi_{hom}(u,w)}. \quad (2.38)$$

Inserting Equation 2.37

$$\hat{\sigma} \approx \frac{\int_{h_u} du \int_{h_w} dw \sigma(u,w)F^0(r)\phi_{hom}(u,w)}{\int_{h_u} du \int_{h_w} dw \phi_{hom}(u,w)}. \quad (2.39)$$

The full-core global homogeneous flux $\phi_{hom}(u,w)$ is approximated by a polynomial expansion or by using hyperbolic basis functions. The full-core global homogeneous flux can be written as,
\[
\bar{\phi}(u, w) \approx \bar{\phi}^{\text{hom}}(u, w) + \sum_{r=u,w} \sum_{l=1}^{L} Q_{l}^{r}(u, w) a_{l,u,w},
\] (2.40)

where

L is the order of expansion,

\( \bar{\phi}^{\text{hom}} \) is the node-average homogeneous flux,

\( Q_{l}^{r}(u, w) \) is the direction-dependent basis functions, and

\( a_{l,u,w} \) is direction-dependent expansion coefficients.

Substituting Equation 2.40 into Equation 2.39, the homogeneous nodal cross-section expression, we have

\[
\bar{\sigma} \approx \int_{h_{u}} du \int_{h_{w}} \sigma(u, w) F^{0}(u, w) [\bar{\phi}^{\text{hom}}(u, w) + \sum_{r=u,w} \sum_{l=1}^{L} Q_{l}^{r}(u, w) a_{l,u,w}] dw
\]

After expanding the above expression and a bit of algebra, the above expression can be written as

\[
\bar{\sigma} \approx \int_{h_{u}} du \int_{h_{w}} \sigma(u, w) F^{0}(u, w) \bar{\phi}^{\text{hom}} dw + \sum_{r=u,w} \sum_{l=1}^{L} \int_{h_{u}} du \int_{h_{w}} \sigma(u, w) F^{0}(r) Q_{l}^{r}(u, w) a_{l,u,w} dw
\]

(2.41)

The basis functions have the property that:

\[
\sum_{l=1}^{L} \left[ \int_{h_{u}} du \int_{h_{w}} Q_{l}^{r}(u, w) dw \right] a_{l,u,w} = 0.
\] (2.42)

Consequently, the homogenised nodal cross-section becomes

\[
\bar{\sigma} \approx \int_{h_{u}} du \int_{h_{w}} \sigma(u, w) F^{0}(u, w) \bar{\phi}^{\text{hom}} dw + \sum_{r=u,w} \sum_{l=1}^{L} \int_{h_{u}} du \int_{h_{w}} \sigma(u, w) F^{0}(u, w) Q_{l}^{r}(u, w) a_{l,u,w} dw
\]

\[
\int_{h_{u}} du \int_{h_{w}} \bar{\phi}^{\text{hom}} dw
\] (2.43)

where \( \int_{h_{u}} du \int_{h_{w}} dw \bar{\phi}^{\text{hom}} = h_{u} h_{w} \bar{\phi}^{\text{hom}} \). Following some rearrangement, we have
Important, we assume that the heterogeneous cross-sections used to compute these moments are independent of the local environmental conditions. This leads to:

\[
\bar{\sigma} \approx \frac{1}{h_u} \int_{h_u} du \frac{1}{h_w} \int_{h_w} \sigma(u, w) F^0(u, w) dw + \frac{1}{\phi_{\text{hom}}} \sum_{r=u,w} \sum_{l=1}^{L} \frac{1}{h_u} \int_{h_u} du \frac{1}{h_w} \int_{h_w} \sigma(u, w) F^0(u, w) Q^l(u, w) a_{u,w}^l dw \tag{2.45}
\]

Equation 2.45 can be rewritten as

\[
\bar{\sigma} = \frac{1}{h_u} \int_{h_u} du \frac{1}{h_w} \int_{h_w} \sigma(u, w) F^0(u, w) dw + \frac{1}{\phi_{\text{hom}}} \sum_{r=u,w} \sum_{l=1}^{L} R_{u,w}^l a_{u,w}^l, \tag{2.46}
\]

where

\[
R_{u,w}^l = \frac{1}{h_u} \int_{h_u} du \frac{1}{h_w} \int_{h_w} \Sigma(u, w) F^0(r) Q^l(u, w) dw, \tag{2.47}
\]

where

\[ R_{u,w}^l \] are the radial homogenisation moments and
\[ a_{u,w}^l \] are the direction-dependent expansion coefficients, determined from the nodal solution.

Since \( F^0 \) is the zero current single assembly radial flux form function, \( \sigma(u, w) \) is the heterogeneous cross-section used in the single assembly lattice calculations and \( R_{u,w}^l \) are the predetermined basis functions. The cross-section radial re-homogenisation moments can be pre-computed by the lattice code and can be presented as functions of the various state parameters.

Equation 2.46 can be rewritten as

\[
\bar{\sigma} \approx \bar{\sigma}^0 + \Delta \sigma^{\text{rehom}}, \tag{2.48}
\]

where

\[
\sigma^0 = \frac{1}{h_u} \int_{h_u} du \frac{1}{h_w} \int_{h_w} \sigma(u, w) F^0(r) dw, \tag{2.49}
\]
\[ \Delta \sigma^{rehom} = \frac{1}{\phi_{hom}} \sum_{r=u,w} \sum_{l=1}^{L} R_{u,w}^{l} a^{l}_{u,w}. \]  

(2.50)

When re-homogenisation moments are used to compute the cross-section homogenisation corrections, the type of basis function expansion employed to generate the moments must be known. In this work the cross-section will be generated via the Legendre cross-section moments from the lattice code.

With Expression 2.48, we can now formulate a scheme for iteratively correcting the nodal cross-section during the nodal calculation. In practice, the cross-section correction is performed at the cross-section feedback iteration level (outermost level in the iterative scheme). The iterative solution would continue until \( \Delta \sigma^{rehom} \) converges to within a set tolerance.

It can be noted that colourset (multi-assembly) homogenization is also sometimes used to generate required nodal parameters. However, a colourset can be computationally unwieldy, because it calls for the simulation of each unique set of four assemblies surrounding the assembly of interest and will appear throughout the reactor core life (Palmtag, 1997). In this work therefore, nodal parameters are generated from a single assembly calculations.

### 2.7 Recent Developments

A number of strategies have been proposed to account for environmental effects on the homogenised parameters. For instance, embedded lattice calculations have been proposed (Mondot, 2003; Ivanov et al., 2008; Colameco, 2012; Colameco et al., 2014) based on the iterations between nodal and lattice calculations. To ease the calculational burden of these embedded calculations, a semi-heterogeneous method in the nodal core analysis was been developed (Groenewald et al., 2017). In this method, the embedded transport calculations are performed, with simplified handling of spatial heterogeneity, energy representation and the order of the solution operator.

Recently, Gamarino et al. (2018) proposed two methods; one in which spatial re-homogenization
of nodal cross-sections is performed using the variation in the 2-D intra-nodal distributions of the few-group flux and net current between the core environment and the infinite-lattice approximation. This method uses on-the-fly variation in the 2-D intra-assembly flux distribution between the core environment and the infinite-medium approximation. The second method he proposes, builds upon spectral re-homogenization to predict the impact of local density changes on the nodal cross-sections. The variation of the infinite-lattice condensation spectrum from a nominal state to a perturbed condition is computed to estimate the variation in cross-sections.

2.8 Conclusions

In this chapter we started off by introducing the NTE which is the basis for reactor analysis. We established that the solution to the transport equation is involved and computationally time consuming. We reviewed the various assumptions and simplifications that ease the solution of the NTE as applied in the deterministic calculational path.

The deterministic path starts off with a lattice calculation. For a given fuel assembly, detailed 2D neutron transport calculations in fine energy group structure are performed, obtaining the heterogeneous flux. To avoid repeating this calculation every time, these 2D, lattice depletion, multi-group transport theory calculations are performed for each assembly type, at several depletion points and expected physical conditions in the core, with materials zones characterized by fine-group cross-sections.

Reflective boundary conditions are applied effectively rendering the lattice transport problem equivalent to the one involving an infinitely large core composed of a single assembly type. In the actual core environment however, an assembly can be surrounded by assemblies of different types, or similar assemblies of different materials, (different burn-up for instance).

Although other boundary conditions can in principle be applied, the reflective boundary condition is considered to represent a more realistic approximation of the in-core environment.
It should be noted here that it is very difficult to reproduce the actual core environment because of the following reasons:

- Due the flux shape, fuel assemblies burn non-uniformly - leading to different material types
- Some assemblies, especially fuel are shifted around from time-to-time leading to different burn-up states.

There are far too many combinations of the reactor states that impact on the environmental conditions that it is not possible to model each and very one of them. Nevertheless, the reflective boundary condition is a reasonable approximation because in general most fuels assemblies, with the exception of a few cases, are placed next to other fuel assemblies.

The lattice calculation provides flux-volume weighted homogenised cross-sections and other equivalent parameters like the diffusion parameters, discontinuity factors, flux form functions, leakage currents etc, generally described as equivalent parameters. These equivalence parameters are defined in such a way that component-average reaction rates and surface-averaged net leakages are preserved when the global multi-group diffusion equation is subsequently solved. The equivalent parameters also help to reduce the subsequent full core calculation cost in terms of time and computer memory.

It was established that although the equivalence theory handles most of the errors due to approximations in the pathway, the environmental error still persists. This is because the cross-sections for loadable assemblies (assemblies that are moved around the core from cycle-to-cycle) are regenerated in infinite lattice (approximate) environments. In general, the real core environment is significantly different from these approximate environments.

This error can be addressed using the re-homogenisation scheme which tries to adjust the infinite lattice environment cross-section to match the real environment cross-section in the diffusion calculation. The scheme is implemented in the global calculation, where the global parameters are determined. The suitability of the scheme in any configuration depends on the severity of infinite lattice cross-sections moments and the basis functions.
In the next chapter, we will develop the procedure to test the scheme for research reactors.
Chapter 3

Methodology

3.1 Introduction

In this chapter, we describe the procedure followed to analyse the environmental error encountered in various research reactor set-ups. The set-up are displayed using models. We use the models to test the re-homogenisation mechanism as implemented in the OSCAR-4 code system. As stated in Chapter 1, this scheme was developed for power reactors and we now want to test it for research reactor designs and in particular for the SAFARI-1 research reactor.

In the first section of this chapter we describe the various codes used in the work. This is followed by a description of the procedure followed to estimate the environmental errors associated with research reactor operations. Lastly, we describe the construction of the various models used.
CHAPTER 3. METHODOLOGY

3.2 Code Systems

Two primary nuclear reactor analysis codes are used in this work, namely OSCAR-4 (Stander, Prinsloo, Muller and DI, 2008) and Serpent (Leppänen, 2011), (Fridman and Leppänen, 2011). Additionally, an internally developed OSCAR-4-Serpent link (Erasmus et al., 2015) was used for data processing from Serpent to OSCAR-4.

3.2.1 Serpent

Serpent is a 3D continuous energy Monte-Carlo lattice physics code whose applications include group constant generation and spatial homogenisation for deterministic reactor simulation calculations. Serpent was developed at the VTT technical research centre in Finland followed by a public release in 2009. Ever since its release, there has been a growing Serpent user community, with more than 28 countries and over 100 organisations using the code across the world. Serpent is currently being used in different nuclear fields including group constant generation, fuel cycle studies, full-core Monte-Carlo reactor modelling as well as in multi-physics calculations (Calic, 2017).

An OSCAR-Serpent pre- and post-processor called the OSCAR-Serpent link, has been developed at Necsa. This tool helps in creating correct Serpent input files for various assemblies and various reactor configurations. It is also used to extract important data i.e. equivalent parameters, as discussed in Section 2.3.7, transferring them in the correct OSCAR-4 format for use in downstream calculations. This setting up of input files and extraction of data is a very involved and error prone process. The tool provides an opportunity to isolate and quantify some of the environmental errors inherent in the deterministic path. The cross-sections and other equivalent parameters are processed using the tool, into the form accepted in the OSCAR-4 system.

For this work, the OSCAR-Serpent link was used to generate homogenised, energy group collapsed cross-sections for components in their correct environments. The Serpent calculations
are considered as the reference solutions since the calculations are done with components in their correct environment.

### 3.2.2 OSCAR-4 code system

OSCAR-4 is the code system that was developed and used by the Radiation and Reactor Theory (RRT) Section at Necsa for the calculational support of the SAFARI-1 reactor. Amongst others, the OSCAR-4 system is used to simulate the day-to-day operations and perform safety analysis for the reactor. The system is currently going through further development so that it can support more reactor designs and incorporate more reactor computation codes for more flexibility.

OSCAR-4 as a code system, consists of several independent codes, each with a specific function. It employs the methods (Section 2.3.2), utilising transport solvers for spatial homogenisation and spectral condensation and then acts as a full-core nodal diffusion solver for the global solution. It consists of a 2D lattice code called the HEterogeneous Assembly DEpletion code (HEADE), a 3D nodal diffusion solver for global core simulation called Multi-Group Reactor Analysis Code (MGRAC), and other utility codes (Stander, Prinsloo, Muller and Tomašević, 2008).

HEADE is a low order collision probability transport solver, utilises a response matrix formalism to solve a 2D fine-group transport problem for a given assembly type (Joubert, 1992). It is used to produce multi-group homogenised diffusion parameters using a 172-group nuclear data library (based on JEFF 2.2) in either WIMS-E or WIMS-D format. Standard unit assembly calculations are utilized to determine homogenized diffusion parameters for fuel assemblies, while colour-set environments are used to determine control rod, irradiation rig and reflector nodal equivalent parameters. HEADE supports both cylindrical and Cartesian geometry types, allows various symmetry options to be defined. Both eigenvalue as well as fixed source calculations are supported.

HEADE produces a set of multi-group homogenized diffusion parameters for use in the global
diffusion calculation. These parameters include assembly averaged cross-sections (the user can control the number and structure of the energy groups), but further also a number of advanced equivalence parameters, such as cross-section moments, pin power/flux form factors and discontinuity factors. These parameters allow for features such as cross-section re-homogenization and flux/power reconstruction in the diffusion solver. The user has the option to select any number of isotopes to be treated microscopically, with the remainder lumped into a single macroscopic structural material.

Infinite models for fuelled elements (i.e fuel and fuel-follower) are modelled in HEADE. This is done to allow microscopic burn-up and state dependent cross-sections to be used for the fuel models, since these cannot as yet be generated through the OSCAR-Serpent link. The HEADE based fuel models are generated with reflective (infinite) boundary conditions around each element. The replacement of fuel cross-sections with these infinite fuel lattice cross-sections, introduces the environmental error associated with the fuel assemblies, as discussed in Section 2.5. The infinite fuel cross-section replacements then allow us to quantify the environmental error as well as to analyse the effect of applying re-homogenisation, as shall be discussed shortly.

The diffusion parameters are fitted against state parameters such as burn-up, fuel and moderator temperature, moderator density etc., for each component type. This fitting is done by a separate utility code called POLX. POLX fits multiple quadratic polynomials to the few-group homogenised cross-section data so as to produce continuous representations of the data. Homogenised cross-sections for all the core components are integrated into a single run-time cross-section library by the utility code called LINX.

The OSCAR-4 system also houses a nodal diffusion solver called MGRAC. MGRAC is the primary code used to simulate the operation of the SAFARI-1 reactor cycle. MGRAC performs global (3D, full-core) multi-group nodal diffusion and depletion calculations using the Multi-group Analytic Nodal Method (MANM) ([Vogel 1992](#)), as the primary solution method. MANM is a variant of ANM as discussed in Section 2.3.6. In this work, MGRAC is used for the nodal core calculations. The “core” in this work refers to the model under
review. The detail of the models are given later in this chapter.

Figure 3.1 shows the schematic representation of the calculational processes followed in OSCAR-4 including the underlying codes utilised at each stage as well as the problems size encountered at each stage. While the CROGEN suite handles assembly size calculations, the CORANA suite handles core wide calculations.

3.3 General Procedure

To evaluate the impact of the re-homogenisation mechanism, some simplified SAFARI-1 representative models are developed. The models are divided into two broad categories i.e. mini-core models and full-core models. The mini-core models consist of two nodes, such as a fuel element and a water box placed side by side.

Figure 3.2 is a flow diagram of the procedure followed in evaluating the re-homogenisation mechanism. Firstly, for each model, a 2D Serpent lattice calculation is performed to generate
the required few-group nodal diffusion parameters required by the nodal diffusion solver, MGRAC. These Serpent calculations provide the reference solutions since all the assemblies are modelled in their correct core environments.

![Flow diagram depicting how the calculations are performed](image)

**Figure 3.2:** Flow diagram depicting how the calculations are performed

The OSCAR-Serpent tool is then used to convert the required parameters into data compatible with the OSCAR-4 system so that subsequent calculations can proceed. The cross-
sections are then used in an equivalent calculation in MGRAC. Equivalence theory, discussed in Section 2.4 is applied in generating these cross-sections, we expect the results from Serpent and the “equivalent” MGRAC calculation to be exactly the same.

The MGRAC calculation is then repeated after replacing fuel cross-sections with homogenised cross-sections from the infinite lattice environment, introducing an environmental error. Cross-sections in the infinite lattice environment are also generated using the equivalence theory but using a different environment to that of the core. Therefore we are intentionally (out of necessity) breaking equivalence and can no longer expect results in MGRAC to be equivalent to the reference Serpent calculation.

The difference in k-eff between the equivalence solution and this infinite environment solution provides an indication of the environmental error introduced.

The MGRAC calculation is repeated again, this time with the re-homogenisation cross-section correction mechanism switched on, taking note of the new k-eff and power distribution (for full-core calculations). At this stage we can evaluate the effectiveness of the re-homogenisation scheme for each model by noting the k-eff changes for the nodal solution.

This procedure gives us three important results, namely:

1. Affirmation that our models are set-up correctly and our calculation path functions correctly when equivalence is obtained between the reference Serpent and reference MGRAC,

2. An estimate of the environmental error associated with the use of homogenised cross-sections from an infinite fuel lattice on a nodal calculation, and

3. A measure of the extend to which the re-homogenisation scheme corrects this error for research reactor type core designs.

We reiterate here that the re-homogenisation scheme was designed for large homogeneous reactors like power reactors which have a low susceptibility to environmental effects. The scheme was extended to research reactor designs like the SAFARI-1 research reactor.
3.3.1 SAFARI-1 facility overview

SAFARI-1 is a 20 MW tank-in-pool type research reactor. Figure 3.3 shows the top (x-y) view of the SAFARI-1 core. The SAFARI-1 reactor core has a checker-board configuration of plate-type fuel elements, control elements and several different types of reflector elements. It is composed of a 9×8 grid filled with various assemblies. It has 26 fuel elements and 6 control elements of the follower type. SAFARI-1 uses follower-type control assemblies, where an MTR type fuel element is attached to the bottom of each absorber element. It is composed of 15 fuel plates centred inside an aluminium frame beneath the cadmium absorber section. The core is reflected by beryllium elements on three sides with one side (with no beryllium reflectors) directly facing the reactor pool. It also has 9 in-core irradiation positions of which 7 are used for Mo-99 production and the other two are used for general isotope irradiation.

![Schematic representation of the SAFARI-1 research reactor](image)

Figure 3.3: Schematic representation of the SAFARI-1 research reactor

3.4 Models

As mentioned in Chapter 2, fuel assemblies are generally moved around the core. As a result, any fuel assembly will have very different neighbours at different times during its duration in the core e.g. next to other fuel assemblies of various burn-up states, next to control
assemblies, next to irradiation positions, or next to control rods (fuel-follower or absorber section). To identify the cases where the scheme may be of value, mini-core models, detailed in Section 3.4.2 are investigated first. Several typical mini-SAFARI-1 environments on which to test the scheme are modelled. Furthermore the scheme was also tested on a full SAFARI-1 core, to quantify the overall impact of the scheme on the global full-core level.

Due to the smaller neutronic size of fuel assemblies, (as opposed to LWR assemblies for power reactors) and the more heterogeneous nature of the core layouts of research reactors, it is of interest to quantify the capabilities of the scheme on such cores.

3.4.1 Model construction

The steps followed in the development of the models for the various cases used in this work are consistent with the model development philosophy that has come about with the creation of the OSCAR-Serpent link at RRT, as described in Section 3.2.1.

To understand the effect of re-homogenisation in the various typical SAFARI-1 environments, several mini-core models are investigated. Each of the mini-core models comprises of two nodes i.e a fuelled node either next to another fuelled or next to a non-fuelled node. The mini-core models used in this work are as follows:

1. Fuel assembly placed next to a water-box ($F - W$),
2. Fuel assembly with burnable absorbers, placed next to a water-box ($BA/F - W$),
3. Fuel-follower placed next to a water-box ($FF - W$) and
4. Fuel assembly placed next to a fuel-follower ($F - FF$).

Reflective boundary conditions were used on all the outer edges for the four cases listed above.
3.4.2 Mini-core models

Fuel water (F-W)

The F-W is a particular case where a SAFARI-1 fuel element is placed next to a similar sized channel filled with light water. This is a typical environment in the core as can be seen in Figure 3.3. The figure shows that there is a significant number of irradiation production rigs in the core. The irradiation rigs comprise mostly of water; there are 9 irradiation rigs in SAFARI-1. Furthermore, in the SAFARI-1 core, 5 fuel elements are positioned such that they are facing the pool-side facility.

The SAFARI-1 fuel assembly is a MTR type fuel, which consists of 19 fuel plates interspersed between water. Figure 3.4 shows the X-Y section (top view) of the SAFARI-1 fuel assembly. The element has external dimensions of 7.590 cm × 8.015 cm immersed in a water cell with dimensions of 7.71 cm × 8.1 cm. The axial height of the active part of the fuel assembly is 59.37 cm.

![Figure 3.4: SAFARI-1 fuel assembly](image)
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The fuel itself consists of 19.75 % (by weight) enriched U-Al alloy, generally known as Low Enriched Uranium (LEU). Figure 3.5 shows a top view of the Serpent F-W model.

![Figure 3.5: Schematic representation of the fuel-water model](image)

**Fuel (with burnable absorbers) water (BA/F – W)**

The BA/F-W consists of a similar type fuel as in Section 3.5 above but the fuel has wire-type burnable absorber (burnable poison) elements on the grid-plate (see Fig 3.6).

Burnable poisons are materials that have a high neutron absorption cross-section that are converted into materials of relatively low absorption cross-section as the result of radiative capture. The burnable poisons in the fuel suppress the neutron flux (by neutron absorption) hence modifying the neutron flux and in-turn adjusting the homogenised cross-sections thereof. The burnable absorbers are made of cadmium. There are no burnable absorbers in all the other cases.

This type of fuel assembly with BA is used commonly in research reactors. Although this is not a SAFARI-1 fuel design, it is included in this study because it is expected to produce more severe environmental effects because of a combination of two factors, i.e. the presence of water and the presence of burnable poisons. It is therefore a good test for the re-homogenisation scheme.
Fuel-follower water (FF – W)

In this case, the fuel-follower is placed next to water as shown in Figure 3.8. The fuel-follower has less fissionable material (fuel) than the fuel assembly and hence there is more water and
structure around it, creating a different environment from the fuel-water case above. Figure 3.7 shows the top (X-Y) view of the SAFARI-1 fuel-follower.

![Schematic representation of the follower-water model](image)

Figure 3.8: Schematic representation of the follower-water model

The follower water is also a typical environment in the SAFARI-1 research reactor which become significant in the later stages of any cycle, as the control rods are withdrawn further from the core.

**Fuel fuel-follower (F – FF)**

This is a case where the fuel assembly is placed next to the fuelled part of the control rod. In the SAFARI-1 core, a number of fuel assemblies are situated next to control assemblies, hence a model where fuel next to follower is an important one. Figure 3.9 shows a 2D schematic diagram of the fuel-follower case.

The cases considered above cover a whole spectrum of possible outcomes when the re-homogenisation mechanism is applied. The fuel designs for MTRs are inherently homogeneous. As result, we expect the F – W model, which typically exhibits the homogeneity character of MTR fuels, to be a poor candidate for re-homogenisation. On the opposite end of the spectrum is the F – FF model, which is significantly heterogeneous. We expect this
model to be a better candidate for re-homogenisation. The $\text{BA/F - W}$ is not a SAFARI-1 fuel design but was included on the list, to confirm that the re-homogenisation mechanism works better in the more heterogeneous fuel designs. As mentioned before, this is one of the reasons why re-homogenisation works well in power reactors. The heterogeneity in power reactors is due to, among other things, different fuel enrichments, arrangement of different fuel designs and the use of burnable absorbers.

3.4.3 Full-core models

Applying the same philosophy as detailed in Section 3.4.2, the full SAFARI-1 core model is developed as depicted in Figure 3.3.

A 3D SAFARI-1 Serpent model, based on the engineering description of the reactor components as depicted in Figure 3.3, is developed. From the 3D SAFARI-1 Serpent model, full-core 2D cuts are selected at the core centre line. Two types of 2D cuts are used i.e. All rods in (ARI) and All rods out (ARO) representing the 2 extreme cases for the rod positions. Serpent generated homogeneous cross-sections for all nodes in the 2D cuts are produced using the two cases. Thereafter, various replacements are made so as to quantify the environmental error in each of the selected cases.
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Full-core 2D Serpent calculations for these two full-core 2D slices are performed, in the process generating the set of nodal equivalence parameters for each node (or core-grid component) present in the 2D cut. Given that the core-diffusion model of the SAFARI-1 core is designed on a $15 \times 14$ grid, 210 sets of nodal cross-sections are generated per 2D cut.

The ARO case is used as a base representative 2D cut, from which the majority of the core-diffusion model is constructed so as to retain the radial equivalence characteristics with the original Serpent transport calculation. However, the control rod absorber cross-sections are taken from the ARI case, as these are not present in the ARO case.

The re-homogenisation model is tested on all the above models in a consistent manner.

3.5 Conclusions

To assess the applicability of the re-homogenisation scheme, two major reactor analysis codes were used, namely Serpent and OSCAR-4. Serpent is a 3D continuous-energy MC reactor physics burn-up calculation code recently developed at the VTT technical research centre in Finland. OSCAR-4 is an in-house reactor analysis code system, developed at Necsa. OSCAR-4 contains a couple of lattice codes, one of which is used in this work (HEADE), a nodal diffusion solver (MGRAC), a cross-section data processing and library generation tool. An OSCAR-Serpent link is also used for processing data between Serpent and OSCAR-4.

The re-homogenisation scheme is assessed by comparing the MGRAC solution to reference a solution. In this work, the reference is the correct-environment, heterogeneous MC solution from Serpent.

Various models, representing the typical SAFARI-1 configurations were developed, on which the scheme is tested, are developed in both Serpent and OSCAR-4. The models can be divided into two categories i.e mini-core and full-core models.

From the Serpent calculation, homogenised cross-sections, in the correct environment, are generated. These cross-sections are then transferred to MGRAC and an equivalent calcu-
lation performed. A small difference between these two calculations shows equivalence, indicating the correctness of the models. In the next stage, the cross-sections in MGRAC are replaced by the infinite lattice cross-sections produced in HEADE. The subsequent MGRAC calculation after these infinite cross-section replacements, provide a measure of the environmental error. This MGRAC calculation is then repeated, this time with the re-homogenisation scheme switched on. This final solution again compared to the reference solution provides a measure of how the efficiency of the scheme.

The re-homogenisation scheme was developed for power reactors but its application have been extended to research rector designs, in particular the SAFARI-1 research reactor. SAFARI-1 is a 20 MW tank-in-pool type reactor using plate-type fuel assemblies. It has a checker-board core configuration. To put the re-homogenisation scheme analysis into perspective, a fuel assembly type with burnable absorbers, is used in one of the mini-core models. Although this is not a SAFARI-1 fuel, these types of fuel assemblies are commonly used in research reactor designs.

Chapter 4.1 provides the results for the mini-core models.
Chapter 4

Mini-Core Results

4.1 Introduction

In this chapter we present the results for the various mini-core models, which were developed in Chapter 3. These are, the fuel assembly next to water (F - W), fuel assembly with burnable absorbers next to water (BA/F - W), fuel-follower next to water (FF - W) and lastly the fuel assembly next to fuel-follower (F - FF). The results for the full-core model are presented in Chapter 5.

As discussed in Chapter 1 (Section 1.1), re-homogenisation schemes have their birth and main application in PWR (power) reactor designs. In these designs, assemblies have notable intra-assembly cross-section variation (i.e. different pin types and finger type control assemblies). Furthermore, the assemblies are much longer and therefore the underlying assumption of environmentally independent cross-section shapes is sound. The question in this chapter is whether these characteristics translate to and are sufficiently retained in MTR design cores for re-homogenisation to prove useful.

For each mini-core model, we start by quantifying the environmental error associated with the model. To achieve this, we compare the Serpent reference solution, to the solution from subsequent MGRAC calculations, performed to evaluate the environmental error, as detailed
The subsequent MGRAC calculations are as follow:

- The equivalent calculation (to check model consistency),
- The infinite fuel lattice replacement (quantification of the environmental error) and then finally
- The MGRAC calculation applying the re-homogenisation scheme, which then helps to evaluate the effectiveness of the scheme.

To further evaluate this scheme, we analyse the primary data applied internally by the scheme i.e. spatial cross-section data from the transport solution (from which cross-section moments are determined) and the core flux shape (from which the expansion moments are obtained). In Section 2.6 we established that the correction factors are estimated using the radial re-homogenisation moments and the flux shape function (see Equation 2.47).

In each mini-core, we estimate the expected re-homogenisation correction by analysing both cross-section and flux shapes from the lattice solution. We extract this data from HEADE output files. Together with other information, HEADE generates few-group (in this case, 6 energy groups) homogenised absorption cross-sections and power maps. This data is produced on a 2D fine mesh, from which 1D profiles can be produced by averaging the data in each transverse direction. For each model we therefore present 1D cross-section and flux profiles processed from the data obtained from HEADE.

HEADE does not generate flux maps directly. We therefore make use of the available power maps as a proxy for flux. Since we are mainly interested in the flux shape, which is quite similar to power shapes, the power profiles provide sufficient information.

The 1D profiles are plotted separately in the two directions indicated in Figure 4.1 i.e. along the fuel plates in the assembly (in the direction denoted “x”) and across the fuel plates (in the direction denoted by “y”).
CHAPTER 4. MINI-CORE RESULTS

4.2 Fuel-Water (F − W) Model

Table 4.1 shows the k-eff values for a F − W mini-core model. The table shows that the difference between the Serpent reference solution and the MGRAC equivalent calculation is about 1 pcm. This confirms the equivalence between the heterogeneous solution and the nodal diffusion solution. It is important to establish equivalence between the two calculations so that only the environmental error remains when fuel cross-sections generated in the correct environment are replaced by those from the infinite lattice environment. This ensures that the environmental error is properly isolated.

Table 4.1: Quantification of the environmental effect in the fuel-water model

<table>
<thead>
<tr>
<th></th>
<th>k-eff</th>
<th>Diff (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Serpent (reference calculation)</td>
<td>1.17033</td>
<td></td>
</tr>
<tr>
<td>MGRAC (equivalent calculation)</td>
<td>1.17032</td>
<td>-0.7</td>
</tr>
<tr>
<td>MGRAC (infinite fuel environment)</td>
<td>1.14294</td>
<td>-2046.9</td>
</tr>
<tr>
<td>MGRAC (with re-homogenisation correction)</td>
<td>1.13671</td>
<td>-2526.5</td>
</tr>
</tbody>
</table>

Table 4.1 also shows that the infinite fuel replacements in the MGRAC calculation intro-
duces about 2 000 pcm error. This difference compared to the reference solution is the environmental error introduced into this model when the fuel cross-sections are replaced.

We reiterate here that in the normal day-to-day reactor operations, correct environment fuel cross-sections are usually not available because of fuel movements described in Section 2.5. Infinite lattice replacements are therefore necessary in reactor simulations. The infinite lattice environment is a practical approximation for the core fuel environment, in the absence of the correct environment. The environmental error thus introduced by cross-section replacement is indeed quite large. The 2 node mini-core is therefore a very severe case to consider i.e. a fuel assembly next to water.

The table also shows that the MGRAC calculation with re-homogenisation correction increased the error by a further 500 pcm to about 2 500 pcm. This means that the scheme failed to correct or even reduce the environmental error in this model set-up.

In summary, Table 4.1 shows the following:

1. There is equivalence between the heterogeneous Serpent calculation and the homogeneous MGRAC calculations. It means that all possible sources of error ranging from modelling mistakes to errors due to the various approximations and simplifications (dealt with through the equivalence theory) were effectively eliminated.

2. A significant environmental error was introduced in the model when correct environment fuel cross-sections were replaced by fuel infinite environment cross-sections.

3. The re-homogenisation schemes failed to reduce the environmental error for this particular model. The error actually grows when the re-homogenisation scheme is applied.

It would have been better to generate the infinite lattice cross-sections in Serpent, for consistency. However, HEADE was used because Serpent had not yet been developed for generating cross-sections for infinite lattice calculations. HEADE was therefore the best alternative. Furthermore, it is noteworthy that the re-homogenisation scheme was developed for infinite lattice calculations. The theory used in the re-homogenisation correction has not yet been extended to colorset (or multi-node) lattice calculations. This implies that we have no choice
CHAPTER 4. MINI-CORE RESULTS

but to use the infinite lattice case as our "wrong" representative environment when applying re-homogenisation.

To understand why the scheme fails in the \( F - W \) model, we analyse the spatial cross-section and flux shapes used by the re-homogenisation scheme in this mini-core model.

Figure 4.2 shows neutron absorption cross-section profiles for the infinite fuel lattice environment and the core (Fuel-Water) environment. As mentioned in Chapter 2, the re-homogenisation mechanism attempts to correct the infinite environment cross-sections to match the core cross-sections. In this case the scheme attempts to match the infinite fuel lattice cross-sections to the Fuel-Water cross-sections.

![Cross-section Profile for F-W in the x-direction](image)

**Figure 4.2**: 1-D macroscopic absorption cross-section profiles for the \( F - W \) mini-core across fuel plates

We make two important observations from Figure 4.2. First, there is a significant off-set between the infinite fuel lattice cross-sections and the core (fuel-water) cross-sections. The off-set widens towards the right hand side (the water side of the mini-core). It is clear that the presence of water creates an environment which significantly differs from the infinite lattice environment. The underlying assumption in the re-homogenisation scheme is that the cross-section shapes are independent of the environment. If this assumption is not severely
violated, one can correct for the average cross-sections by weighting the cross-section shape with the core (correct) flux shape. From Figure 4.2 the significant cross-section shape difference indicates that this assumption is violated, hence this case is a poor candidate for re-homogenisation.

Secondly, the cross-section profile from the infinite lattice shows very little shape variation. While the core profile decreases along the x-direction, the infinite lattice profile is symmetric about the centre of the fuel assembly. The off-set described above is therefore much wider than the variation in the infinite lattice profile. As a result, there is very little room for any weighting function (flux-shape) to produce significant corrections to the infinite lattice cross-sections.

Homogenised cross-sections are flux-volume weighted, hence the flux profile give us an indication of the weighting function used. Although we have already established in this case that no weighting function will adjust the infinite cross-section to match the core cross-sections, we nevertheless have a look at the flux/power profile for the case.

![Figure 4.3: Power profile for the F - W mini-core across fuel plates](image)

Figure 4.3 shows the power profiles along the x-direction. As stated in Section 4.1 power distribution is used in this work as a proxy for flux. The core (fuel-water) flux is used as a weighting function to recompute the homogenised cross-sections. This function shows
some potential to correct the cross-sections. However, the variation in this profile, is not enough to adjust for the significant off-set we saw in the cross-section shapes in Figure 4.2. Considering Equation 2.40, the weighting function is made up of two parts i.e the zero\textsuperscript{th} order term (average flux) and higher order expansion terms. The cross-section correction factor is computed using the higher order terms since the zero\textsuperscript{th} order term is assumed to cancel (eq.2.50). What this means is that if the off-set in the cross-sections (Fig.4.2) is considerable, there is no cross-section correction, because correction factors in the higher order terms do not contribute sufficiently to the computation of homogenised cross-sections. It is for the above reasons that the re-homogenisation scheme fails in the fuel-water mini-core.

A similar analysis for the 1D profiles in the y-direction i.e. across fuel plates, is performed here.

Figure 4.4 is a plot of the cross-sections in the y-direction. The figure shows that the off-set in the cross-sections is much wider in the y-direction than in the x-direction, which might mean that much of the contribution to the environmental error comes from the y-direction. However, the two profiles are quite similar and the off-set is constant across the fuel plates. In the same way, as described above, there is very little chance that any weighting function can correct for these cross-section differences. The weighting function for this case is shown in Figure 4.5.

Figure 4.5 is the power (flux shape) profile in the y-direction. The two profiles are almost identical, which means that in the nodal diffusion calculation the homogenised cross-sections are computed using the same weighting function as used in the transport calculation, hence the correction factor is almost negligible.

It can be seen from the above discussion that the violation is more severe in the y-direction than in the x-direction where there are significant flux shape differences (Figures 4.2 and 4.4). The cross-section moments and flux shape functions are perturbed more in the x-direction because of the water box in this direction. However, the off-set in the cross-sections is so significant that the small cross-section correction in the x-direction does not result in a reduction in the assembly wide environmental error.
CHAPTER 4. MINI-CORE RESULTS

Figure 4.4: 1-D macroscopic absorption cross-section profiles for the F – W mini-core along fuel plates

Figure 4.5: Power profile for the F – W mini-core along fuel plates
In summary the re-homogenisation scheme fails in the \( F - W \) model. This is because the cross-section difference between the infinite lattice environment and the core environment is much greater than the infinite cross-section shape variation. Thereby the weighting function cannot correct for such an error.

### 4.3 Fuel-Water with Burnable Absorbers (BA/F – W)

Table 4.2 shows the k-eff values for the fuel-water mini-core with burnable absorbers in the fuel side plates (BA/F – W). Due to the presence of burnable absorbers, the reference solution is sub-critical with a k-eff of 0.99217, compared to the reference solution for the F-W case. The equivalent MGRAC solution shows very good equivalence at 2 pcm error. The infinite environment introduces a 6 700 pcm difference. The re-homogenisation correction significantly reduces this difference down to about 2 500 pcm. This therefore means that the re-homogenisation cross-section correction mechanism reduced the error by about 4 300 pcm.

The above analysis shows that the homogenisation correction mechanism works very well in this type of environment. We will take a look at the underlining mechanism to understand why the scheme works in this case. As mentioned in Section 3.4.2, this is not a standard SAFARI-1 assembly but it was included in this work to illustrate the typical example of a case where the re-homogenisation scheme can significantly reduce errors.

Table 4.2: Quantification of the environmental effect in the fuel (with burnable absorbers) water mini-core model

<table>
<thead>
<tr>
<th></th>
<th>k-eff</th>
<th>diff (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Serpent (reference calculation)</td>
<td>0.99217</td>
<td></td>
</tr>
<tr>
<td>MGRAC (equivalent calculation)</td>
<td>0.99215</td>
<td>-2</td>
</tr>
<tr>
<td>MGRAC (infinite fuel environment)</td>
<td>1.06296</td>
<td>6712</td>
</tr>
<tr>
<td>MGRAC (with re-homogenisation correction)</td>
<td>1.01775</td>
<td>2533</td>
</tr>
</tbody>
</table>

Figure 4.6 depicts the cross-section profiles across the fuel plates in the (BA/F – W) model.
The figure shows a major increase in the absorption cross-sections on the edges of the fuel element. Neutron poisons (i.e. burnable absorbers) have a large neutron absorption cross-section, hence their presence increases the average absorption cross-section in that region. Next to the burnable poisons the absorption cross-section drops sharply only to increase significantly again in the middle section of the fuel assembly. This shape variation is somewhat reproduced in the other side of the fuel assembly.

The infinite lattice cross-sections in the figure are generally higher than BA/fuel-water cross-sections indicating the error introduced due to infinite lattice replacements. Looking at the figure again we see that the underlying assumption is again violated. There is a shape difference between the infinite lattice and the core cross-sections.

![Cross-section Profile for BA/F-W in the x-direction](image)

**Figure 4.6:** 1-D macroscopic absorption cross-section profile for the BA/F – W mini-core along fuel plates

However, the shape variation (described above) in the infinite fuel lattice cross-sections is more pronounced than the off-set. For instance the off-set is about 20 % and the shape variation spans over an order of magnitude in cross-sections. A significant shape variation in the infinite lattice cross-sections means that a different weighting function has the potential to produce improved homogenised cross-sections, hence there is room for cross-section cor-
CHAPTER 4. MINI-CORE RESULTS

The extent of the correction then depends on the shape of the weighting function (flux shape) used.

Figure 4.7 shows the infinite lattice and the mini-core flux shape. The mini-core flux shows a slight variation along the fuel plates. However, because of the cross-section variations in Figure 4.6, the small variation in the weighting function produces significant cross-section changes.

![Power Profile for BA/F-W in the x-direction](image)

Figure 4.7: Power profile for the $BA/F - W$ mini-core along fuel plates

Figures 4.8 and 4.9 show the cross-section and flux profiles for the $(BA/F - W)$ mini-core in the y-direction. As we have seen previously, the y-direction is not perturbed and hence there is not much variation in that direction. This again shows that there is very little contribution to the cross-section correction from the y-direction.

4.4 Fuel-Follower Water (FF – W) Model

Table 4.3 shows the results for the fuel-follower water (FF – W) mini-core model. The k-eff of 1.09124 for the reference solution is lower than the reference solution for the (F – W)
Figure 4.8: 1-D macroscopic absorption cross-section profile for the $\text{BA/F - W}$ mini-core across fuel plates

Figure 4.9: Power profile for the $\text{BA/F - W}$ mini-core across fuel plates
model. This is because the fuel-follower has fewer fuel plates than the fuel assembly. There is less fissionable material, hence the follower is less reactive.

At 3 pcm reactivity difference between the MGRAC and the Serpent calculations shows good equivalence with the reference solution. Again the finite environment introduces a significant error of about 3 000 pcm. The homogenisation correction mechanism again fail to correct the error, in this case as evidenced by the further increase in the error by about 800 pcm.

Table 4.3: Quantification of the environmental effect in fuel-follower mini-core model

<table>
<thead>
<tr>
<th></th>
<th>k-eff</th>
<th>diff (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Serpent (reference calculation)</td>
<td>1.09124</td>
<td></td>
</tr>
<tr>
<td>MGRAC (equivalent calculation)</td>
<td>1.09121</td>
<td>-3</td>
</tr>
<tr>
<td>MGRAC (infinite fuel environment)</td>
<td>1.05608</td>
<td>-3051</td>
</tr>
<tr>
<td>MGRAC (with re-homogenisation correction)</td>
<td>1.04797</td>
<td>-3784</td>
</tr>
</tbody>
</table>

The re-homogenisation mechanisms fails in the same way as described in Section 4.2. Since the fuel-follower is quite similar to the fuel assembly although sightly smaller, we expect it to behave in much the same way.

4.5 Fuel Fuel-Follower (F – FF) Model

The (F − FF) model is markedly different from the the previous models. While the previous models were composed of a burnable element next to water, in this case we have two burnable elements next to each other. This creates a significantly different environment. The results for the fuel-follower mini-core environment are shown in Table 4.4.

The k-eff for all the calculations for this case shows very high reactivity due to the presence of larger amounts of fissile material i.e. in both the follower and the fuel. The reference k-eff at 1.634707. The table shows that the fuel infinite environment introduces a small environmental error worth 201 pcm. As mentioned earlier, an element in an infinite environment is
Table 4.4: Quantification of the environmental effect in the fuel and fuel-follower mini-core model

<table>
<thead>
<tr>
<th></th>
<th>k-eff</th>
<th>diff (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Serpent (reference calculation)</td>
<td>1.63407</td>
<td></td>
</tr>
<tr>
<td>MGRAC (infinite environment -both components)</td>
<td>1.62872</td>
<td>-201</td>
</tr>
<tr>
<td>MGRAC (re-homogenisation on fuel)</td>
<td>1.62777</td>
<td>-237</td>
</tr>
<tr>
<td>MGRAC (re-homogenisation on follower)</td>
<td>1.62997</td>
<td>-153</td>
</tr>
<tr>
<td>MGRAC (re-homogenisation on fuel and follower)</td>
<td>1.62902</td>
<td>-190</td>
</tr>
</tbody>
</table>

Akin to the element being surrounded by an infinite lattice of similar elements. The fuel next to the fuel-follower mini-core is closer to this infinite environment than the other mini-core cases reviewed. Since the fuel-follower environment is closer to the infinite, the cross-section replacement produces a small error.

Table 4.4 also shows the results where the re-homogenisation scheme is switched on selectively. When the scheme is switched on in fuel, the error worsens to 237 pcm. This is consistent with what we saw in the fuel-water case. The fuel assembly is very homogeneous such that the cross-section movements do not have enough room for correction even in an improved environment like we have in this case. However, when the scheme is switched on in both the fuel and the follower, the error is reduced from 201 pcm to 190 pcm. This improvement is attributed to the follower assembly. The follower assembly is smaller and has more non-fuel structure around it. The cross-section shape is more pronounced because of the structure around it, hence there is more room for cross-section correction. When the scheme is switched on in the follower assembly only, the error is reduced further to 153 pcm. The fuel-follower is therefore a very good candidate for re-homogenisation.

This noted improvement in the follower is an important result, as it identifies an area of potential improvement in the SAFARI-1 model. The result also confirms our observation that re-homogenisation only add value where the cross-section moments have sufficient shape to offset the underlying assumption that the moments themselves are independent of environ-
4.6 Verification

For this work, the aspect of verification is inherent in the procedure followed. All the various mini-cores discussed in this chapter, and the full-core, discussed in Chapter 5, are modelled in both Serpent and OSCAR-4, where the Serpent results are considered as reference. The code-to-code comparison between the k-eff from the reference solution and the k-eff from nodal diffusion solver helps verify that the models are correct and consistent. In all the cases, this comparison showed a very small difference in the reactivity, thereby confirming that the models were correctly and consistently constructed.

4.7 Conclusions

The re-homogenisation cross-section correction mechanism is designed to adjust the infinite lattice cross-sections in the nodal diffusion solver to match the real environment cross-section using the cross-section moments obtained from the lattice calculation.

The re-homogenisation scheme is tested in the following mini-core models; \((F - W)\), \((BA/F - W)\), \((FF - W)\) and \((F - FF)\). We managed to quantify the environmental error associated with these various SAFARI-1 mini-core environments.

The results show that the re-homogenisation scheme fails in the \((F - W)\) and the \((FF - W)\) models. The underlying assumption in the re-homogenisation scheme, that the cross-section shapes are independent of the environment is violated in these models. In these two cases, the difference in the cross-section shape is much wider the correction-effect of the cross-section moments. The overall result for these two case is that the solution worsened.

However the scheme reduces the environmental error in the \((F - FF)\) and the \((BA/F - W)\) cases. Although the underlying assumption is also violated in these cases, the violation is not
as severe. The (F - FF) is an important case in the SAFARI-1 reactor core. The SAFARI-1 core has 6 control assemblies. This case is particularly significant towards the end of cycle where fuel-followers gets inserted into the core. The (BA/F - W) is not a SAFARI-1 design but it indicates typical case where the scheme is supposed to work.

In the next chapter, we show the results of the full SAFARI-1 model and investigate the impact of the re-homogenisation scheme on the full-core calculations.
Chapter 5

Full-Core Results

5.1 Introduction

The effects of the infinite fuel approximation and subsequent use of the re-homogenisation correction mechanism in OSCAR-4 were further evaluated using a full-core, 2D ARO case, with fresh fuel assemblies. Since SAFARI-1 uses fuel-follower type control assemblies, ARO in this case means that all six control positions are occupied by fuel-followers. In Chapter 4 we saw that the mechanism showed potential in the model where fuel was placed next to fuel-followers. This case is also explored further in the full-core model.

Full-core means calculations are performed on a core arrangement similar to the one used for SAFARI-1 operations. However, the core configuration used in this model is slightly different from the one used for commercial purposes. For instance, all the irradiation positions for isotope and molybdenum production were modelled as empty. These empty rig positions then represent the typical fuel-water case analysed in Chapter 4.

In this case, we will use both reactivity and full-core power distribution to quantify the accuracy of the re-homogenisation scheme. We consider the average and the maximum power produced.
As per our procedure, we start off by comparing the Serpent (reference) solutions to the subsequent MGRAC calculations. The infinite fuel replacement, with and without re-homogenisation finally gives us a measure of the effectiveness of the scheme in this model.

### 5.1.1 Global results

Table 5.1 shows reactivity, the average power error and the maximum power error as obtained in the global SAFARI-1 All Rods Out core with fresh fuel assemblies.

<table>
<thead>
<tr>
<th>Model</th>
<th>Error (pcm)</th>
<th>Avg. Power Error (%)</th>
<th>Max. Power Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference (from Serpent)</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>MGRAC (equivalent)</td>
<td>-74</td>
<td></td>
<td></td>
</tr>
<tr>
<td>MGRAC (infinite fuel)</td>
<td>252</td>
<td>2.30</td>
<td>4.49</td>
</tr>
<tr>
<td>MGRAC (re-homogenisation)</td>
<td>88</td>
<td>1.69</td>
<td>3.52</td>
</tr>
</tbody>
</table>

The table shows the difference in k-eff between the Serpent reference solution and the equivalent MGRAC calculation is 74 pcm. We notice here that this error in the equivalent calculation for the full-core case is somewhat higher than is obtained in all the other mini-core models analysed. However, the error is still small enough to signify equivalence. It is not surprising that this error, at the full-core level is higher, because of the numerous combinations of errors through-out the core. As the problem gets bigger, the errors due to modelling approximations increase as well, hence the bigger error in the equivalence calculation for full-core.

The table also shows that when correct core cross-sections are replaced with infinite fuel environment cross-sections, an environmental error of 252 pcm is introduced. This error is much smaller than the infinite environment error for mini-core models. It is important to consider that the mini-core cases are quite extreme in nature e.g. a fuel assembly next to
a water channel. The environment in this example is much different from the environment
where the replacement cross-sections are obtained from and thus the environmental error
introduced is quite substantial.

In the full-core model however, many more fuel elements have other fuel elements as neigh-
bours and so the infinite lattice approximation is much more reasonable. In practice, the
environmental error is often primarily induced from neighbour burn-up differences, which is
exactly the kind of environmental errors that the re-homogenisation scheme was developed
for. Be that as it may, a fresh core was used for quantification in this case. Although this
error is small, it still shows that using cross-sections from the infinite environment into the
real core introduces an environmental error, even on a full-core.

Table 5.1 also shows that the equivalent calculation introduces a 4.49 % maximum power
error and a 2.30 % average power error. When the re-homogenisation mechanism is applied,
the error in k-eff is significantly reduced from 252 pcm to 88 pcm. The maximum power
error goes down to 3.52 % while the average power error also goes down to 1.69 %.

These results show that the re-homogenisation scheme improves the accuracy of the nodal
solution in the full-core calculation. The re-homogenisation mechanism significantly reduced
all the errors in the three parameters used here i.e. k-eff, average and maximum power.

Although the scheme appears to be working well on the full-core level, it is important to
evaluate whether it works in all the positions. As mentioned earlier, MTR type reactors
are heterogeneous such that various positions in the core might behave quite differently.
Furthermore, since in the previous chapter we isolated some potential candidates for re-
homogenisation to work well, it is necessary to evaluate how these candidates perform in the
full-core case. To this end, we analyse the power distribution in the core. Each assembly
which contains fissile material, contributes a certain fraction to the 20 MW produced in the
core. This power distribution is discussed in the next section.
5.1.2 Power distribution

In this section, we analyse the power distribution for the full-core model. Figure 5.1 shows the full-core relative power distributions in the SAFARI-1 full-core.

The figure only shows the relevant part of the SAFARI-1 core for this study i.e. it does not show reflector assemblies since they do not produce power. The 10 core positions (in blue) do not have fuel and therefore no power is produced there. As stated above, a core-configuration with empty irradiation rigs was used. The control assemblies i.e the places occupied by fuel-followers, are indicated with a red outline. The control assemblies are in positions C5, C7, E5, E7, G5 and G7.

In each assembly there are two numbers. The top number is the reference calculation power fraction for each assembly in this configuration. For example, position B3 produces 2.57 % which is approximately 514 kW. The number at the bottom in each assembly is the relative error in the power obtained when infinite fuel lattice cross-sections are introduced. In other words, this number indicates the environmental error introduced by the cross-section replacements. It should be noted that since the total power is maintained at 20 MW, introducing the approximate environment may reduce the power fraction in some elements, resulting in power increase in other elements. As a result, the relative power errors can either be positive or negative. A positive error value represents an increase in power fraction whereas a negative value represents a reduction in the power fraction.

From Figure 5.1 we see that the maximum power produced in a single fuel assembly is 4.65 % of the 20 MW produced in the SAFARI-1 reactor configuration and this maximum power is produced at position E6. This position is situated in between control rod positions. In general, the figure shows that the fuel assemblies situated in between control rod assemblies produce significantly higher power than the other fuel assemblies.

The figure shows that the infinite fuel approximation introduces significant power errors in positions C5, C7, E5, E7, G5 G7 including positions C6 and D7. These positions have errors above 3.2 %. While the first six are control rod positions (fuel-followers), the last
Figure 5.1: Assembly averaged relative power fractions for the reference ARO case with relative power errors for the infinite fuel approximation two are positions adjacent to the followers. This result confirms our observation that the environment around control assemblies produces significant environmental effects.

We analyse the errors further after a MGRAC calculation applying re-homogenisation. The success of the scheme is measured by the reduction of the power error.

Figure 5.2 shows the relative power distributions similar to the one shown in Figure 5.1. The relative power (top number) is reproduced from Figure 5.1. However, the bottom number in this case indicates the power error when the re-homogenisation scheme is applied. By comparing the previous power error to the current power error we can identify the positions where the scheme improves the nodal solution and where it gets worse. The table shows that the re-homogenisation scheme reduces the power error in most of the positions. It can be seen that the highest error reductions are in the fuel-followers where the environmental error introduced by the infinite fuel environment almost halved when re-homogenisation is applied.

It can be seen therefore that the re-homogenisation in the research reactor environment, particularly in SAFARI-1, could be quite valuable in the control rod assemblies where the
CHAPTER 5. FULL-CORE RESULTS

Figure 5.2: Assembly averaged relative power fractions for the reference ARO case with relative power errors for the infinite fuel approximation with re-homogenisation en-
vironmental error tends to be large.

Figure 5.3 is the SAFARI-1 core map depicting the effectiveness of the re-homogenisation scheme in the case under consideration. On the map, red represents positions were the nodal solution worsened, green represents the place where it improves and grey represents the places where the solution remains largely the same.

The figure shows that most fuel positions, with exception of those closely matching an x-direction fuel-water configuration (i.e C4, E4 and G4), mildly improve or stay constant. The other x-direction fuel-water configurations have followers around them, hence this negative effect is somewhat suppressed.

The H-row shows mixed behaviour, as the cross-section moments (shape functions) are less pronounced in the y-direction and hence re-homogenisation has a smaller impact. Column 4 shows a clear deterioration for fuel adjacent to the empty rig (fuel-water) case. It is however interesting that Column 7 does not share this deterioration. This is largely due to
the overriding improvement from the neighbouring follower elements. It is also interesting to note that there are various places where the scheme reproduced the infinite environment error i.e. the error neither got better or worse. These indifferent positions concentrated towards row H.

It seems evident that re-homogenisation can be used in this core design. However, it could be of value to switch the scheme off in the particular fuel-water environments where it deteriorates the solution.

Although the mechanism did not improve all the mini-core solutions analysed, it significantly improves the results on a full-core scale, which is what we are interested in. We note that the mini-core cases represent only a small subset of fuel positions. In particular, cases such as row H or Column 4 (the typical fuel-water type cases) or the control rod positions (C5, C7, E5, E7, G5 and G7) can easily be related to these cases. The rest show much milder environmental variation, where we expect good improvement from re-homogenisation.

Two important observations can be drawn from the results thus far. First, considering the structure of fuel assemblies, we see that the effect of homogenisation is direction dependent. The x-direction shape function dominates the correction factor. The second observation is

![Figure 5.3: Re-homogenisation scheme map](image)
that, the severity of the $F - W$ case as detailed in the previous chapter, is still quite evident, even in the full-core case.

Considering these two preliminary observations, we can expect re-homogenisation to improve the solutions further, if we selectively apply it. The strategy is to switch the scheme off in all the fuel-water cases.

As a way of further analysis, the MGRAC calculation was repeated with re-homogenisation switched off in the fuel-water cases as proposed.

From this selective position switching calculation the average power error improved further from 1.69% to 1.61%. Figure 5.4 shows the power errors after the re-homogenisation scheme was switched off in select positions matching x-direction fuel-water environment.

<table>
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<td>3.83</td>
<td>2.16</td>
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<tr>
<td>D</td>
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<td>3.73</td>
<td>4.42</td>
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<td>1.36</td>
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<tr>
<td>E</td>
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<td>3.34</td>
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<td>2.60</td>
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<tr>
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<td>4.38</td>
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<td>3.54</td>
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<td>2.23</td>
<td>2.47</td>
<td>2.33</td>
<td>2.09</td>
<td>1.29</td>
</tr>
</tbody>
</table>

Figure 5.4: Assembly averaged relative power fractions with relative power errors for re-homogenisation scheme selectively switched off

Figure 5.5 shows the core map again with the re-homogenisation scheme switched off selectively in some places. Figures 5.4 and 5.5 show a further improvement of the errors. The scheme improves the results in most of the positions. Only three positions are worsened.
It is however quite interesting that when re-homogenisation is selectively applied, there was a significant rise in the number of “indifferent” positions from 4 to 8.

It seems that further investigation into dynamic position and directionally dependent re-homogenisation scheme could hold some promise and is proposed as a possible continuation of this work. At this stage, we simply propose the various core environments are evaluated on a case-by-case basis to determine in which positions the scheme should be applied.

**Figure 5.5:** Re-homogenisation scheme map with re-homogenisation scheme selectively switched off

### 5.1.3 Conclusions

We introduced an environmental error in the full-core MGRAC calculation for SAFARI-1 by introducing fuel cross-sections from an approximate (infinite lattice) environment. We quantified this error by comparing to the reference Serpent calculation. The environmental error due to infinite approximation was 252 pcm, 2.30 % in average power and 4.59 % in maximum power. We further quantified the capability of the re-homogenisation scheme to reduce these errors by applying the scheme in the subsequent MGRAC calculation. The scheme reduced these errors to 88 pcm, 1.69 % and 3.52 % respectively.
It was observed that the overall benefit of the re-homogenisation scheme applied to the full-core calculation can be improved if the scheme is used selectively to avoid the core positions where re-homogenisation does not apply. It was noted that the x-directed fuel-water case consistently worsens the error. Further calculations to selectively switch off the scheme in these cases were performed. These results showed further improvement with the average power error going down from 1.69 % to 1.61 %. It was noted that cross-section correction moments are direction dependent because of the structure of fuel assemblies (plate-type). However, switching off the scheme in particular directions is beyond the scope of this work.
Chapter 6

Conclusions

The suitability of the re-homogenisation cross-section correction scheme was hereby analysed and quantified. The scheme was developed for power reactors and is now being used in research reactor designs.

The deterministic calculational path, used in the modelling and simulation of nuclear reactor introduces a number of approximations and simplifications leading to errors in reactors analysis. However, most of these errors are dealt with by the use of equivalence theory. Nevertheless, there still remains a significant source of error in the path; the environmental dependency in cross-section generation. This error comes as a direct consequence of the need to replace correct environment fuel cross-sections with approximate environment fuel cross-sections, giving rise to the environmental error.

In this work, a number of SAFARI-1 reactor models were built for the specific purpose of analysing the homogenisation scheme. A number of mini-core models together with a full-core All rods out case were used in this work.

The underlying assumption used in the re-homogenisation scheme is that cross-section shapes are independent of the environment. However, this assumption is violated in most of the cases, even in the cases in which the scheme improved the error. The results show that the more severe cross-section shape is, the more room there is for the scheme to correct
the error. As a consequence, in the more homogeneous and large mini-cores e.g. fuel-water environment, the scheme failed to correct the error. However, in the more heterogeneous environments e.g. BA/F -W the scheme reduced the error significantly. Although the BA/F -W is not a SAFARI-1 environment, it helped to illustrate the typical environments where the scheme works.

For SAFARI-1, it is quite interesting that the environment in which a fuel-follower is placed next to standard fuel showed a lot of potential. It appears that in the SAFARI-1 case the scheme is particularly useful in the areas around the control assemblies.

This observation was further strengthened in the full-core model where the fuel-followers showed a greater sensitivity to environmental effects than the regular fuel elements. In general, the scheme improved the nodal solution on the full-core environment.

We can conclude that the existing re-homogenisation model can potentially be used in the research reactor environment. However, the scheme has to be used carefully, such that it is only applied in the areas which do not violate too severely its underlying assumptions.

As a result, further work needs to be done to develop a “smart” re-homogenisation scheme. It might be useful if the scheme makes a quick analysis of the underlying cross-section shapes and fluxes before the core calculation is executed (i.e. during the lattice calculation phase). This way, the scheme can be switched on or off, depending on its potential for correction.

6.1 Future Work

Two important observation made in the work may form the basis for the future work that may be carried out, to improve this cross-section re-homogenisation scheme. First, it was noted that the cross-section correction capability of the scheme can be improved if it is applied selectively in the core. The scheme can therefore be improved by incorporating an algorithm which internally switches off the scheme in potentially adverse configurations like the Fuel-Water case.
It was also noted that due to the structure of the fuel assemblies, the correction effect of the scheme is directional. An added capability of switching off the scheme in some directions could prove valuable.
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