

The Development of a Nodal Method for the Analysis of PWR Cores with Advanced Fuels

by

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I hereby declare that the work described in this thesis is that of my own unless clearly stated otherwise.

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Abstract

This thesis outlines the development of a nodal method with the purpose of addressing difficulties encountered in the modelling of advanced fuels. The standard calculational route used when modelling a Uranium (U) fuelled Pressurised Water Reactor (PWR) is not accurate enough to analyse a PWR containing U and Plutonium (Pu). This is because the assumptions made when developing the standard route are not necessarily representative of situations involving advanced fuels.

To address some of these poor assumptions a nodal method has been developed which can solve the SP_N equations in multiple energy groups. The SP_N equations are an asymptotic approximation of the full neutron transport equation, and as such will include more physical effects than the neutron diffusion equation. The theory behind the development of this nodal method is outlined in this thesis along with an extensive set of benchmark tests for verification of the method. It is found that through a similarity transformation of the determining equations, existing nodal diffusion solvers can obtain solutions to the SP_N equations without any approximations.

Previously EDF Energy have developed an embedded methodology to address the shortcomings of the standard calculational route. This procedure solves the diffusion equation in greater detail on local sub-meshes in order to correct the standard 2 group nuclear data, and reduces the pin power errors by $\approx 50\%$ by capturing spectral effects on the interface between two significantly different fuel types. In this thesis the incorporation of the SP_N nodal method into the embedded methodology is described.

A small light water reactor benchmark is solved to test the accuracy of the embedded methodology combined with the SP_N nodal method. It is concluded that similar accuracy to diffusion is attained with the SP_N equations. This is because the homogenisation procedure produces an error larger than the improvements due to the use of the SP_N equations. To address the limitations discovered in this thesis future work is proposed based on the author's experience of research in the area.

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Acronyms

AA Aragones and Ahnert⁵

ANM Analytic Nodal Method

BCGSTAB Biconjugate Gradient STABilised

BOL Beginning Of Life

CMFD Coarse Mesh Finite Difference

CP Collision Probabilities

DF Discontinuity Factor

EDC Effective Diffusion Coefficient

EDF Électricité de France

FD Finite Difference

FEM Finite Element Method

FMFD Fine Mesh Finite Difference

Gd Gadolinium

GET Generalised Equivalence Theory

ILC Infinite Lattice Calculation

KS Smith⁶

LWR Light Water Reactor

MCNH Moon et al.⁷

MOC Method Of Characteristics

MOX Mixed OXide

NEM Nodal Expansion Method

ODE Ordinary Differential Equation

PANTHER Pwr and Agr Neutronics and Thermal Hydraulics Evaluation Route

PARCS Purdue Advanced Reactor Core Simulator

PDE	Partial Differential Equation
PSPN	PANTHER SP_N
Pu	Plutonium
PWR	Pressurised Water Reactor
QUANTM	Quadratic Analytic Nodal Transport Method
RHS	Right Hand Side
SA	Single Assembly
SANM	Semi-Analytic Nodal Method
SPH	SuPerHomogénéisation
UNM	Unified Nodal Method
U	Uranium
UOX	Uranium OXide
WIMS	Winfrith Improved Multigroup Scheme

Chapter 1

Introduction

Developments in reactor core analysis methods have been dictated by a combination of physical constraints such as computational power and speed, and incentives such as the potentially beneficial economics of using advanced fuel designs. These physical and modelling constraints have required great simplification of the problem to be solved numerically, while retaining an appropriate level of accuracy. In this context advanced fuels are those containing Plutonium (Pu) which does not originate from the transmutation of elements within that same fuel.

Historically, commercial Pressurised Water Reactors (PWRs) were fuelled entirely with Uranium OXide (UOX), the only Pu inventory being produced during burnup. This similarity of fuel over such a large area of the core resulted in the neutron density varying smoothly in space, except in the vicinity of pins within individual fuel assemblies. In a situation similar to this, a large near-critical domain which possesses a cellular nearly periodic structure, the solution to the neutron transport equation can be decomposed into a solution to a Single Assembly (SA) Infinite Lattice Calculation (ILC) and a global diffusion calculation⁸. This depends on the solution to the problem of an assembly surrounded by an infinite number of identical assemblies being a good approximation to an assembly surrounded by a finite number of similar assemblies.

This realisation has led to the use of SA ILCs to provide homogenised two energy group data for use in a global diffusion calculation. Additionally, pin power form factors are also computed in the ILCs so that the power at individual fuel pin locations can be reconstructed from the global diffusion solution. The current methods of homogenisation⁹ have been tailored to this idealised setting, which is now being challenged by the introduction of advanced fuels.

It is still the case that due to computational constraints full core heterogeneous calculations cannot be performed for routine reactor analysis, and it is still desirable to retain ILCs on an assembly scale. It has, however, become desirable in practical reactor operation to load core configurations which challenge the assumptions of the early methods. There is now a requirement to model core loadings including both Mixed OXide (MOX) and UOX fuel of various enrichments and burnups.

The introduction of two different yet neighbouring fuel types brings into question the validity of ILCs. Significant heterogeneities in the global solution at the interfaces between different assembly types produce pin power errors in the realm of 10% which are unacceptable to most practitioners. These interface errors produced by the standard calculation route have been extensively studied for cores loaded with MOX and UOX assemblies, and can be attributed to 4 main features^{10–12}.

These new features are: a spatial discretisations error from the difficulties encountered by some numerical methods in modelling the severe flux gradients at the interface between different fuel types; an error in the homogenisation of the cross-sections resulting from the use of an ILC that has no information about the true local core environment; group collapsing (flux weighting cross-sections when collapsing to two groups) errors due to the interface having neither a purely MOX or UOX spectrum; a transport error from the diffusion approximation no longer being sufficient to capture all of the physics occurring at the interface.

The spatial discretisation error has been observed in relation to the Nodal Expansion Method (NEM) which yields unstable solutions, in the presence of severe flux gradients, that are a result of having a polynomial basis. This deficiency can be addressed by using an Analytic Nodal Method (ANM) or Semi-Analytic Nodal Method (SANM) to capture the large gradients seen in the neutron flux¹⁰. This is a result of the flux being expanded in terms of functions which are analytic solutions to certain forms of the diffusion equation.

When a MOX assembly is introduced next to a UOX assembly then the net current on their common interface departs significantly from zero. The Pu in a MOX assembly is highly absorbing compared to Uranium (U), at thermal energies, causing the flow of neutrons into the MOX fuel pin to be higher than that leaving. The flux spectrum on the interface is now neither that of MOX or UOX in isolation. However, in each assembly the cross-sections will have been collapsed into two energy groups in an ILC with flux spectra that differ significantly from that on the interface. A similar effect is seen at the core-reflector boundary where the peripheral assemblies are adjacent to a steel baffle surrounded by water.

Further, the cross-sections are homogenised spatially via flux weighting with the solution from an ILC that has no information about the change in the flux near the MOX-UOX interfaces. The uniform intra-assembly fluxes used for the homogenisation will therefore be unrepresentative and yield inaccurate reaction rates in the global calculation. The whole core diffusion theory solution also differs significantly from that of neutron transport theory at the common interface because it ignores the anisotropy of the angular flux in this region.

This thesis describes a nodal method that has been developed with the aim of correcting some of the errors outlined previously. The main result is a nodal method for an approximate neutron transport model which can capture effects that a diffusion model cannot. This has been combined with a methodology recently developed by EDF Energy that aims to correct

spectral and homogenisation errors arising from the interface between MOX and UOX fuel.

This chapter proceeds by outlining the background theory in section 1.1. The aim is that the reader will understand the current state of the art at the time this thesis is written. It should also give an impression of where the research contained herein fits with the current literature on the topic. In section 1.2 the current approaches to tackle the problems found at these MOX-UOX interfaces are outlined. Section 1.3 details the methodology developed at EDF Energy, section 1.4 the research objectives and section 1.5 is a thesis outline.

1.1 Background Information

In this section a standard calculational scheme for a UOX fuelled core is presented. The specific methods described are those used by EDF Energy, but these are representative of most calculational schemes for PWRs^{13–17}. With this calculational scheme one is only interested in obtaining information about a steady-state (no time dependence). Further, thermal-hydraulics and burnup considerations are also excluded as they are not within the scope of this work.

The scheme starts with the preparation of nuclear data via SA ILCs. Nuclear data is imported from an internationally recognised library such as JEF-2.2¹⁸ into the Winfrith Improved Multi-group Scheme (WIMS). This is a lattice cell code that prepares microscopic cross-section data in many finite energy groups from the nuclear data library. WIMS is also capable of performing neutron transport calculations for explicit geometries in many energy groups with the prepared cross-sections. Once a detailed solution has been obtained for a chosen geometry the code can then use it to collapse the number of energy groups and materials to a few representative macroscopic cross-sections for use in external codes.

As outlined in the previous section WIMS is usually run for each assembly type in the core in an

infinite lattice of identical assemblies, resulting in homogenised cross-sections and discontinuity factors in 2 groups, and pin power form factors. This is all the information necessary to preserve the reaction rates and surface currents seen by that assembly in the ILC⁹. The homogenised cross-sections are computed to preserve the reaction rates and the discontinuity factors are introduced in order to preserve the surface currents. Pin power form factors are also output to allow the spatial reconstruction of the power in the individual pincells within the assembly. These homogenised data are used by a reactor analysis package in a full core calculation in 2 energy groups using neutron diffusion theory. The geometric representation of the core is by now highly simplified with a single set of material properties describing an assembly region.

The resulting solutions obtained using this calculational scheme are found to be highly accurate and within a few percent of the actual pin powers seen in the reactor. It is the introduction of advanced fuels into reactors that has challenged the assumptions that this calculational scheme is based on.

1.2 Current Approaches to Modelling MOX-UOX Cores

An intuitive extension to the single assembly ILC is to cover multiple assemblies in one calculation, a colorset, thus encompassing these troublesome interfaces¹⁹. A larger portion of the core, for example 4 assemblies in a 2x2 grid, could be modelled explicitly capturing the interface between different fuel types. The solution for this larger problem will have the correct spectrum on the interface and shape for the intra-assembly flux. This can then be used to collapse the number of energy groups, and a homogeneous diffusion solution can be obtained for this colorset to ensure that the homogenised cross-sections will preserve the reaction rates. The problem with this approach is the number of lattice cell calculations that would need to be

performed. As fuel is burnt up and shuffled around the core the interfaces would be changed and the computationally expensive lattice calculations would have to be redone at every stage. For this reason this method is not routinely used²⁰.

In order to retain SA ILCs and include the effects of the nearest neighbours various methods have been developed. These all involve sub-models which can approximate the effect of nearest neighbours either during the solution process or prior to it. These sub-models are capable of obtaining a more accurate solution on various scales and for various assembly subdivisions. These sub-models are normally simplified compared to the ILCs by having fewer groups, homogenised regions and can employ diffusion or SP_3 (approximate transport) models²¹, but even heterogeneous geometry transport calculations can be performed¹¹. There are also not necessarily only two levels of calculation, global and local; there can be various intermediate levels in order to accelerate the convergence of the method or obtain an approximate idea of the core environment. These techniques incorporate some of the ideas found in other multi-scale methods¹². The coupling of the sub-model to the global scale is done in various ways which will be touched on briefly in the next section. These sub-models can be used to prepare new, or corrections to, standard few group homogenised cross-sections and discontinuity factors used in the global model.

1.2.1 Specific Examples

The following examples are of methods which have successfully reduced the errors seen in the standard calculational route due to the MOX-UOX interface. They are summarised to illustrate the current state of the art. The descriptions are necessarily brief and the reader is referred to the references to gain an in-depth understanding of the specific coupling methods and simplifications used.

Ivanov¹¹ has replaced the offline method of preparing nuclear data with an online embedded SA calculation. An embedded calculation is one which is performed with a better physical model and/or on a more detailed geometry, but for a subset of the full problem. This is in order to compute a more accurate solution that can capture an effect that is missed in the full calculation. Two methods of solving the embedded problems were investigated. The first was an SP₃ Finite Element Method (FEM) calculation with homogenised pincell data in multiple energy groups and the second was a Collision Probabilities (CP) lattice cell calculation. The coupling between the global and local (embedded) scale is achieved using an albedo boundary condition. The albedo boundary condition is a modified reflective boundary condition that specifies the fraction of the outgoing partial current that is reflected. Using the solution to the embedded problem online computations of discontinuity factors and homogenised cross-sections are performed. This re-computation of homogenised cross-sections is termed cross-section re-homogenisation. The local parameters are then used in a global NEM to obtain updated albedos at the assembly boundaries. This process is then continued until the global problem has converged. The process of iterating between a global and local calculation to obtain a solution has been termed online as opposed to offline which will refer to local calculations performed in advance to provide data for a global calculation.

A three level model has been proposed by Lewis¹² using the SP₃ equations to capture transport effects. This method also uses an online re-homogenisation procedure where the ILC is a pin-by-pin SA multi-group SP₃ problem solved using Fine Mesh Finite Differences (FMFDs). In this method the boundary conditions from the global problem are again imposed in the local problems. The local SP₃ SA calculation is used to provide two group homogenised pincell cross-sections and discontinuity factors. This data is used in an extra layer of local calculation solving pin-by-pin SA two group problems with diffusion theory. The numerical method is

also FMFD and the solution to this problem is used to generate homogenised cross-sections and discontinuity factors for the global Coarse Mesh Finite Difference (CMFD) method. The CMFD method is a technique used to reduce memory requirements and accelerate global high-order calculation methods such as the nodal method. A global CMFD calculation with one node per assembly is then performed in two-group diffusion theory. The computed global interface currents are then expanded using spectral information from the previous iteration and applied as boundary conditions to the SP_3 solution method. The existence of the second local diffusion theory calculation is purely to accelerate the method.

A more advanced nodal method with a consistent pin power reconstruction has been proposed by Palmtag²². The nuclear data is still prepared using the standard route of offline SA ILC. It is the way in which the homogenisation of this data is done that differs significantly. The solution information from the ILC calculations is stored in such a way that it can be easily accessed online. At each power iteration the new global solution is used in conjunction with the offline reference SA solution to compute updated cross-sections and discontinuity factors for each assembly for use in the next power iteration. This method can be thought of as having an offline embedded method, but online cross-section re-homogenisation. Further to this, an empirical spectral correction has been implemented using intra-assembly polynomial cross-section variations.

SIMULATE-5 (derived closely from SIMULATE-4) uses multiple sub-models in order to retain the single assembly ILC^{16,21}. The global solver is a multi-group ANM with homogenised assembly cross-sections and discontinuity factors. There are both an axial and a radial sub-mesh. The axial sub-mesh takes into account leakage and has less to do with the modelling of advanced fuels. The radial sub-mesh constitutes a slice of the whole core with assemblies subdivided following the pincell boundaries. The assemblies in the 2D slice are normally subdivided into

5 coarse meshes constituting a strip around the edge, to capture the interface effects, and a single central region. The material data for each of the 2D slices is obtained from standard SA ILCs. Either a multi-group diffusion or SP_3 solution is obtained for the full radial slice and for each isolated assembly with a zero current boundary. The difference in the two solutions for each assembly is then used to update the cross-sections and discontinuity factors in the global model. This is done online and iteration between the sub-model and global model converges the solution.

Westinghouse has developed a spectral effect model to tie in with their global SANM²³. The conventional homogenised cross-sections and discontinuity factors are corrected using information from the local core environment. This is done by adjusting the discontinuity factors and including a spatial variation in the assembly cross-section which uses the pre-existing inter-assembly burnup gradient treatment. There are not many details available of the precise methods used.

A quasi-diffusion whole core method has been developed by Clarno and Adams²⁰ that uses Eddington tensors to allow direction dependent diffusion coefficients. SA ILCs are still used as in the standard route but an offline method of correction for nearest neighbours is proposed. On a set of sub-meshes, which use explicit transport and diffusion multi-group solvers, a set of 1D interface and colorset calculations are performed. These are approximations to a full colorset calculation and are used to determine a set of albedos which describe the effect of a nearest neighbour. The SA ILCs are then run a second time with the albedos derived from the sub-meshes to determine a set of deviations from the standard methodology. These deviations are for a small reference set of configurations, which through superposition can represent all configurations of assemblies in the core.

The methods outlined above represent a wide variety techniques from completely online to

completely offline computation of corrections to the standard route. The common themes in terms of improvements are more energy groups, a closer approximation to the local core environment, an increase in resolution and cross-section re-homogenisation. The online calculations are expected to be more expensive purely because they extend the amount of time taken to converge to a solution, albeit a more accurate one. Offline methods have the advantage that the online calculation is not impacted. Any approach to the problems posed by advanced fuels is therefore likely to include the generic aspects indicated above, and considerations of the impact on speed and ease of implementation in current calculational routes.

1.3 Current Progress by EDF Energy

The standard calculational route in PANTHER, the EDF Energy reactor analysis code, has been applied and validated for PWR cores with UOX fuel. WIMS is used to perform single assembly ILCs resulting in 2-group homogenised nuclear data². This nuclear data is then used in a whole core neutron diffusion theory calculation using the ANM.

Rather than produce a whole new methodology for modelling cores with advanced fuels, an approach has been developed which involves correcting the current validated methodology. The single assembly ILC is retained, along with the whole core assembly homogenised nodal solution. What is introduced is a third intermediate level of calculations, that, by comparison to the standard single assembly approach, provides corrections to account for the effects seen at MOX-UOX interfaces.

The third level of calculation is designed to capture the interface effects between the different types of assemblies. A set of embedded colorset problems are defined, according to the chosen loading pattern, that consists of four quarter assemblies encapsulating all of the interfaces, in

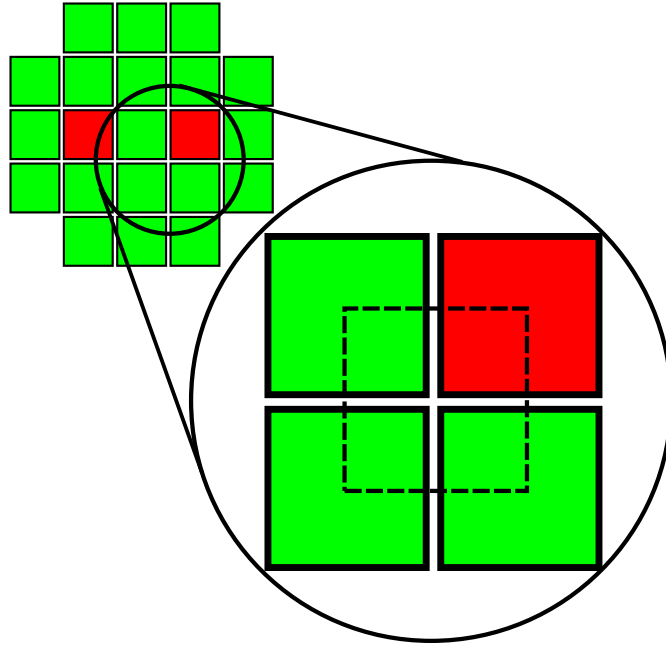


Figure 1.1: The selection of an embedded colorset is illustrated. The behaviour on an interface between two different assembly types, red and green, is captured by modelling the four quarter assemblies in the dashed line.

particular MOX-UOX. This is illustrated in fig. 1.1. The improvement in the solution comes from a pin cell level description in an increased number of energy groups. The single assembly ILC is used to collapse data from 172 energy groups to 6 group pintype data, alongside the standard 2 group smeared data. The 6 group pintype data is then used in these embedded calculations to capture spectral effects which are missed in 2 groups. The choice of embedded colorsets is motivated by Zhanga et al.¹⁹.

Once the embedded colorset calculation has been solved in 6 groups the homogeneous 2 group diffusion solution is obtained. It is the difference between the 2 solutions that allows corrections to be defined to the homogenised data. This technique is based on Bahadir et al.¹⁶ and Shen²⁴. The corrected homogenised data is then used in the whole core 2 group nodal diffusion solution procedure to obtain a more accurate solution. This procedure has a completely offline computation of the corrections, and therefore the impact on calculation time should be minimal.

1.3.1 Preparation of the 6-Group Nuclear Data

It was decided that applying Generalised Equivalence Theory (GET)²⁵ to obtain homogenised pincell cross-sections in 6 groups would produce an impractical amount of data. There would be 4 discontinuity factors per pincell per group as a minimum. Instead flux weighted homogeneous cross-sections were output for each pintype along with the target reaction rates for each assembly. This information can then be used to compute SuPerHomogénéisation (SPH) factors¹⁴ which preserve pintype reaction rates, average leakages and the k_{eff} .

This method of applying SPH factors to pintype data to preserve reference reaction rates has been tested and found to be sufficiently accurate for reactor core calculations^{26–30}. Recently this method has also been applied to the SP_N equations with promising results²⁷. To preserve the quantities of interest only one SPH factor per pintype per group is required as in diffusion. Further to this it has been found that the use of pintype SPH factors is almost as accurate as the use of an SPH factor for each individual pincell, but requires much less data to be stored.

The motivation behind the embedded methodology is to keep the single assembly ILC in WIMS intact. In order for this to be the case the SPH factors are computed within PANTHER as part of the correction procedure. Each assembly is considered in isolation. The 6 group pintype data taken from WIMS is used to construct an ILC calculation with homogenised pincells in PANTHER. The non-linear iteration procedure is used with the reference reaction rates from WIMS to determine the SPH factors. This procedure can be performed in parallel so that the overall impact on execution time is small.

With the SPH factors in hand the colorset problem is then constructed in both the 6 group pin-by-pin and the 2 group homogenised configurations. Corrections to the 2 group homogenised data are then computed based on the differences between the two solutions. The assumption is

that the difference between the 2 and 6 group colorset calculations are representative of those seen in the core on the corresponding interface. What are produced are not only corrected cross-section data, but also corrected discontinuity factors and pin power form factors.

The version of the embedded methodology that has been developed by EDF Energy for the WIMS PANTHER calculational route uses a diffusion model in 6 groups to determine the corrections. The results of using this analysis have recently been published² and are summarised in the next section.

1.3.2 KAIST Benchmark Results for the Embedded Methodology

The KAIST 1A small MOX core with zoning¹ was chosen for this benchmark comparison. Figure 1.2 shows the geometry of the problem. It is a quarter core with an explicit steel baffle and reflector region. There are both MOX and UOX assemblies with explicit models of the fuel pins.

The data has been prepared by setting up SA ILC in WIMS. These are used to extract the 2 group homogenised data and 6 group pintype data. A WIMS model of two assemblies, the reflector and baffle, has been set up to extract reflector data.

Two main comparisons have been performed in order to determine the effects of using the embedded methodology. The first is against a PANTHER pin-by-pin whole core calculation in 6 groups. The second is against a heterogeneous WIMS calculation of the whole core also in 6 energy groups. The first calculation has been performed to determine the errors involved in deriving corrections to a whole core calculation from isolated colorsets. The second gives an idea of how well the method will perform in real-life situations, and how well the 6 group diffusion model can capture the heterogeneous effects.

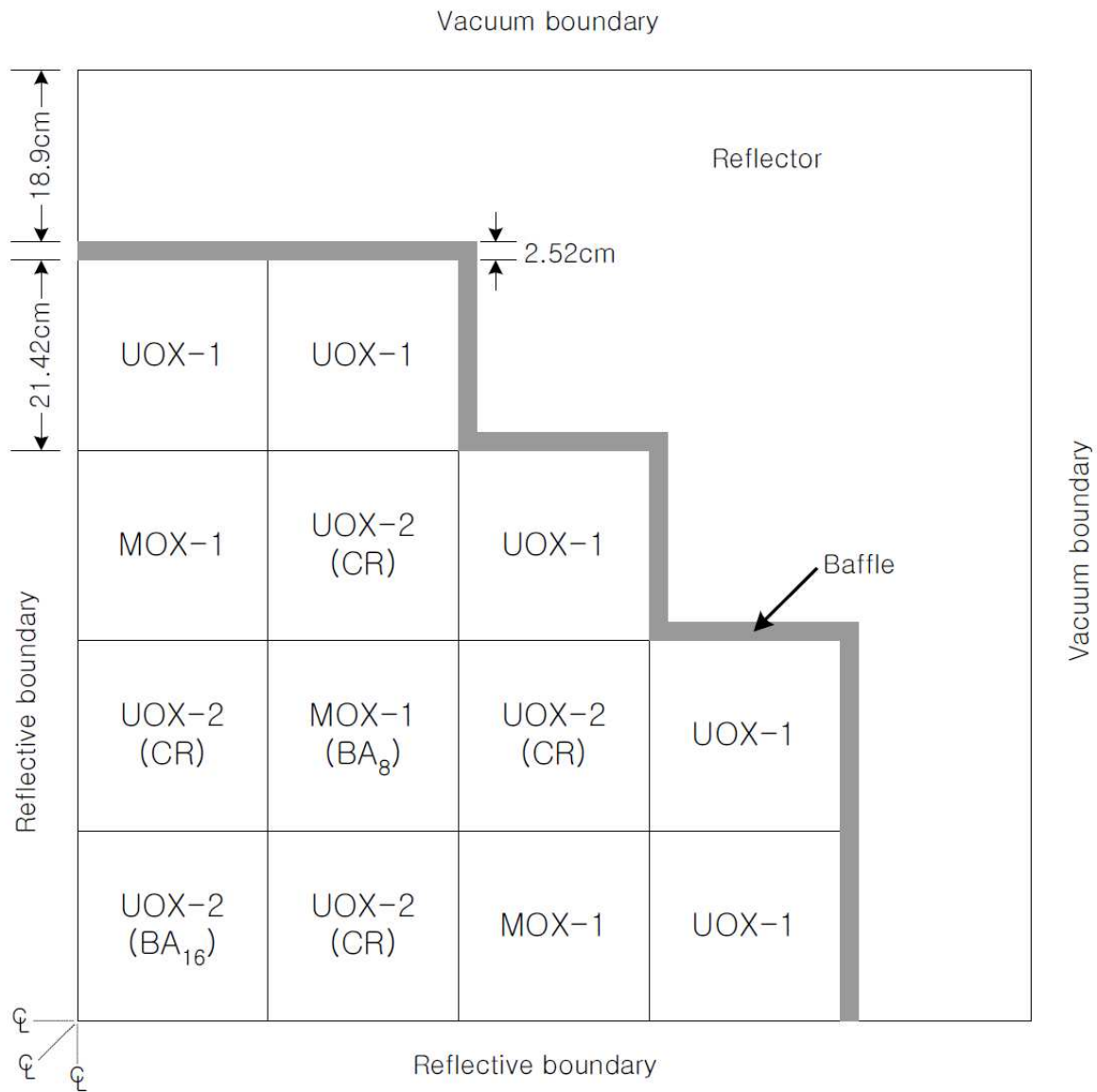


Figure 1.2: Geometry of the KAIST benchmark 1A¹.

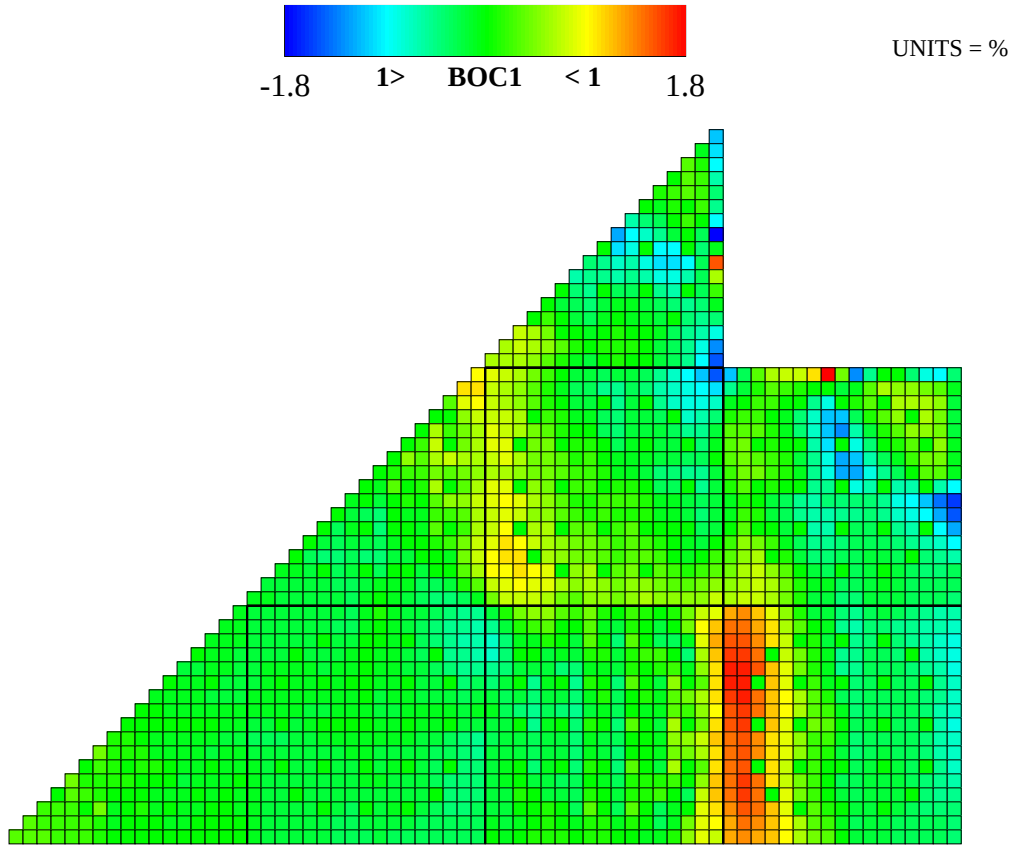


Figure 1.3: Pin power errors when comparing the embedded method against a PANTHER whole core pin-by-pin calculation. Figure taken from Knight et al.².

Pin-by-Pin PANTHER for a Whole Core

As this is primarily a test of the errors due to performing embedded calculations, the single assembly data was taken from PANTHER. This meant that both the embedded solver and the whole core 6 group pin-by-pin solver use the same physical model and data. The difference is that the embedded colorset calculations are lacking the boundary leakage information when computing the corrections for use in the whole core 2 group homogeneous diffusion calculation. The reconstructed pin powers from the 2 group homogeneous diffusion calculation are then compared against the whole core 6 group pin-by-pin calculation. The errors in the pin powers are shown in fig. 1.3 and a summary of the results in table 1.1. It should be noted that the Gadolinium (Gd) pin powers have been excluded from the comparison as their size are negligible.

Table 1.1: Results of the comparison between PANTHER pin-by-pin and the embedded methodology, taken from Knight et al.². SA is the standard single assembly route and EMB is the embedded route. BOC stands for the beginning of cycle when the core is loaded exclusively with fresh fuel. The unit of reactivity used here is the millinile (mN).

Model	Burnup	Channel Power Error (%)			Pin Power Error* (%)			k_{eff} (mN)
		RMS	min	max	RMS	min	max	
SA	BOC1	1.02	-2.1	1.5	1.59	-4.8	7.7	192
EMB	BOC1	0.20	-0.2	0.4	0.35	-0.8	1.2	-11

* pin power errors are given for all pins with a relative power greater than 0.7

These results are very encouraging as the errors have been reduced to under 2% for all powers. Further to this a large improvement is seen in the prediction of the k_{eff} . The embedded methodology is able to reproduce the results from a whole core calculation while reducing the errors in the standard calculational route.

Heterogeneous WIMS Calculation in 6 Groups

For this comparison a heterogeneous geometry model of the whole core is produced and a CP calculation is performed to collapse all the nuclear data to 6 groups. Using this 6 group data and the heterogeneous geometry the Method Of Characteristics (MOC) is used to provide the reference powers and k_{eff} . In addition to this SA ILCs are performed using the MOC to provide homogenised data for PANTHER and the embedded route. The data generated here for the embedded methodology is exactly the same as that used in the pin-by-pin whole core calculation. This means the embedded methodology will give exactly the same solution as in the previous section. The differences between the two sets of errors shown are therefore due to effects that cannot be captured by the embedded methodology.

The results are shown in fig. 1.4 and summarised in table 1.2. The pin powers errors are reduced by a factor of 2-3 when compared to the standard route. The k_{eff} is also improved compared to the WIMS reference.

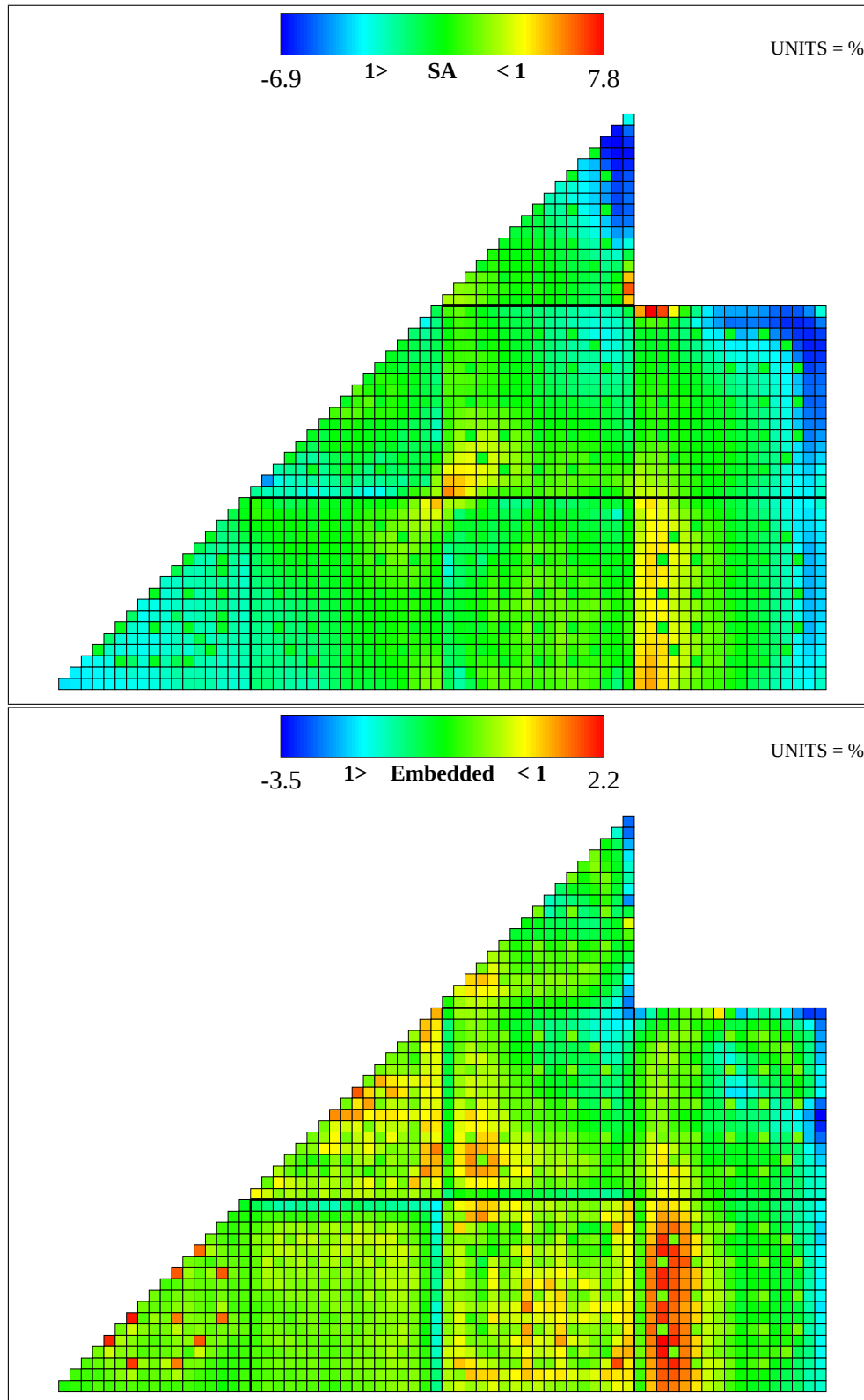


Figure 1.4: Pin power comparisons against a heterogeneous WIMS reference. The top figure shows the results for the standard route and the bottom for the embedded route. Taken from Knight et al.²

Table 1.2: The results of a comparison against a 6 group heterogeneous model solved with WIMS. These results were initially reported in Knight et al.².

Model	Burnup GWd/te	Chan Pow Err (%)			Pin Pow Err* (%)			k_{eff} (mN)
		RMS	min	max	RMS	min	max	
SA	0	0.94	-2.2	1.4	1.54	-4.7	5.8	158
EMB	0	0.36	-0.6	0.5	0.63	-2.1	1.8	-46

* pin power errors are given for all pins with a relative power greater than 0.7

Summary of the Benchmark Results

The predictions of pin powers by the embedded methodology show a significant improvement over those of the standard calculational route. What has been shown is that much of the error in the standard route is a result of using too few energy groups to capture the complicated spectral effects between assemblies of different types. What is interesting is that a diffusion model is sufficient to capture this level of detail and that corrections can be precomputed, meaning that whole core calculations retain their existing efficiency.

The residual errors, $\approx 3\%$ in the pin powers, are due to the homogenisation of the data, and the lack of knowledge of the correct boundary conditions for each embedded colorset calculation and effects that cannot be captured using a diffusion model. It is the last of these errors that are addressed in this thesis. The basic idea is to use an approximate neutron transport model, such as the SP_N equations, to solve the embedded colorset calculations and define corrections for use in whole core calculations. What are not in the scope of this thesis are radical changes in the lattice cell calculations and the data extracted from them. The background work which has provided motivation for the research described in this thesis has now been outlined. In the following section the research objectives for this thesis are outlined.

1.4 Research Objectives

Considering the title of the thesis, the first objective is to develop a nodal method capable of solving the SP_N equations. Nodal methods have been chosen due to their proven computational efficiency and accuracy in solving elliptic Partial Differential Equations (PDEs) on coarse domains. Both the neutron diffusion equation and the second-order SP_N equations can be solved numerically using nodal methods and there is some experience of doing this in the literature which has been crucial in developing the method presented here.

The second objective involves integrating the methods developed, as part of the first objective, into the embedded methodology from EDF Energy. The third objective is to quantify the accuracy of the embedded methodology, with the integrated SP_N nodal method, when solving problems involving advanced fuels. The problems which will form the focus of this thesis are those involving cores loaded with both UOX and MOX fuel as this is the most studied and widely used advanced fuel.

1.5 Thesis Outline

This thesis is broadly divided into two parts. The first part is the development of an SP_N nodal method along with details of the implementation and benchmarking. The second part details the integration of the SP_N solver into the embedded methodology. This is then applied to benchmark problems to draw conclusions about the effect of using the SP_N equations in this context.

In chapter 2 the SP_N equations are derived and transformed into a form that a nodal method can be applied to. Further mathematical details are also given and derivations of the boundary

conditions. These results are new to the field and have been published in a peer reviewed journal article³⁹. Chapter 3 describes the nodal method chosen to solve the SP_N equations and the reasons behind this. The nodal method is generally applied within the framework of the CMFD method and this is detailed in chapter 4. A specific form of the CMFD method is derived for the SP_N equations and some preliminary results are presented. In chapter 5 the results of a comprehensive set of benchmarks are described confirming that the accuracy of the SP_N nodal method is as expected.

Chapter 6 describes the preparation of the nuclear data for use with the SP_N equations within the embedded methodology, and the results of its application. A simple problem of a line of UOX and MOX pincells is considered to determine the impact of homogenisation on an interface between the different fuel types. The homogenisation procedure used to correct for transport effects and reproduce pin powers in SA ILCs is then extended to the SP_N equations. Once these important preliminary results have been obtained the embedded methodology is applied to a colorset and quarter core calculation to determine the efficacy of the embedded methodology with an SP_N nodal method. The main results of this thesis are then summarised with the conclusions in chapter 7 and recommendations are given for further research.

Chapter 2

The Simplified Spherical Harmonics Equations

The information presented in chapter 1 has highlighted the problems inherent in the use of advanced fuels, and the ways in which these have been addressed by various researchers. In this chapter progress towards developing an approximate neutron transport solver are described. There has been a large amount of renewed interest in utilising the SP_N approximation for reactor physics applications^{3,16,29,31–34}. Many reactor analysis codes now include an SP_N option and some use it for production calculations²¹. The reason for using the SP_N equations over diffusion theory, for reactor core calculations, is to include some of the transport effects seen at the interfaces between Mixed OXide (MOX) and Uranium OXide (UOX) assemblies.

Due to the proven efficiency of nodal methods for the numerical solution of the neutron diffusion equation they have been employed to solve the SP_3 equations in various codes^{12,16,31,33,35,36}. This extension is possible by a simple transformation from the original form of the SP_3 equations, with coupling between the angular moments on the diffusion terms, to one that resembles the multi-group diffusion equation. The scattering term in the multi-group equations is transformed

from a group-to-group to a pseudo group-to-group scattering matrix where some of the “groups” correspond to angular moments. The only extension to $N > 3$, for a nodal method, that the author is aware of is attributable to Smith³⁶ in the code Quadratic Analytic Nodal Transport Method (QUANTM).

As the SP_N equations are an asymptotic approximation to the full P_N equations there is no general rule for determining the order at which to truncate them. The full P_N equations will converge to the exact transport solution as additional moments are included, but this is not true of the SP_N equations. There is no definitive order at which the SP_N approximation should be terminated and it is beneficial to have an accurate and efficient method to compute higher-order solutions to investigate this. It is for this purpose that the SP_N nodal method presented in this work was developed. The approach adopted in this thesis is an extension to existing SP_3 nodal methods. A transformation is used to map the SP_N equations into a multi-group neutron diffusion like form. It is then possible to apply a nodal method to this system of equations to obtain a solution.

A more general form of the mapping is known and has been used previously in solvers of different types^{37,38}. It is believed by the author that this chapter outlines some mathematical properties of the transformed SP_N equations that have not been reported before. These properties guarantee that the pseudo group cross-sections are positive in general. This means that any multi-group diffusion solver, including a nodal method, is capable of solving the SP_N equations without adaption.

The work described in this chapter is a slightly modified form of a paper that has been published in the Annals of Nuclear Energy³⁹. This chapter briefly mentions the justification for using the SP_N equations in section 2.1 and then a derivation of the equations is presented in section 2.2. The extension to the boundary conditions is given in section 2.3.

2.1 Theoretical Justification

The SP_N equations were first derived as an *ad hoc* approximation to the P_N equations by Gelbard⁴⁰. This involved taking the first-order form of the P_N equations in slab geometry and swapping the derivative term in 1D with a divergence operator in the even-order equations and a gradient operator in the odd-order equations⁴¹. This approximation yielded surprisingly good results (greater than 80%⁴² of transport corrections to the diffusion equation) for some reactor analysis problems, but was not used due to little available theoretical justification. In relatively recent years two excellent papers were published on the theory of the SP_N equations^{37,43}. These two papers present separate asymptotic expansions that result in the SP_N equations. Both papers show that the SP_N equations are a high-order asymptotic expansion of the P_N equations with the leading-order equation being a neutron diffusion model.

Larsen et al.³⁷ showed that the SP_N equations are a higher-order asymptotic correction to diffusion theory. This was done by making assertions about the relative sizes of the cross-sections in a given problem. The main physics implied by this scaling is:

- The system is optically thick $\Sigma_t \gg 1$, where Σ_t is the total cross-section.
- The rate of absorption and production are comparable and weak.
- The neutron diffusion equation is invariant under this scaling.

Pomraning⁴³ showed that the SP_N equations are asymptotically related to the slab geometry P_N equations. If a local reference frame exists that has a 1D character, with respect to the geometry and solution, then a good approximation can be obtained. This is better illustrated with the example shown in fig. 2.1. This geometry is taken from Brantley and Larsen³ and has 3 fuel plates embedded in a moderator that is inside a vacuum. The pseudo 1D nature of the problem can be clearly seen. Neutrons travelling along the x -axis see a very transport dominated

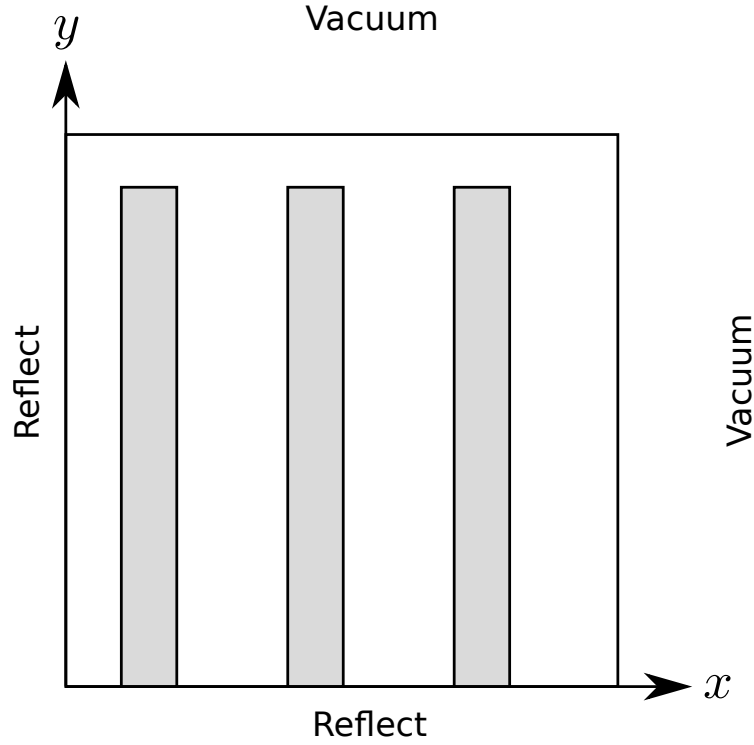


Figure 2.1: This is the geometry of a test problem taken from Brantley and Larsen³. There is a pseudo 1D character that can be well approximated with the SP_N equations, except at the tips of the fuel plates.

problem, whereas neutrons travelling along the y -axis see an almost homogeneous medium. This is not true at the tips of the fuel plates where the problem has a very heterogeneous nature.

If a given problem does not display either of these features then there is no guarantee of the accuracy of the solution, and in fact the solution can be worse than diffusion. There are also situations in which the SP_N equations are equivalent to the P_N equations⁴¹. These are: an infinite domain in 3D with a constant total cross-section and isotropic source(s); in 1D cylindrical or spherical geometry with linearly anisotropic sources and scatter.

Although the asymptotic analyses give some insight into the types of problems that can be successfully solved, a practical set of criteria has not been laid down. The most convincing argument for the application of the SP_N equations, as an approximation of the P_N equations, in reactor physics is the improvement seen when applied to realistic problems. Significant reductions in error are observed in the pin-powers and reactor eigenvalue.

2.2 Multi-Group Diffusion Form

In order to write the SP_N equations in the form of the multi-group neutron diffusion equations, it is necessary to begin with the within-group neutron transport equation in slab geometry with isotropic scattering and sources,

$$\left[\mu \frac{\partial}{\partial x} + \sigma(x) \right] \psi(x, \mu) = \frac{q(x)}{\sqrt{2}}, \quad (2.1)$$

where $\psi(x, \mu)$ is the angular flux, $\sigma(x)$ is the total cross-section, μ is the cosine of the polar angle and $q(x)$ is an isotropic source containing fission and scatter contributions. The factor of $1/\sqrt{2}$ comes purely from the definition of q and is introduced to simplify notation later. The even-parity angular flux is defined as

$$\psi^+(x, \mu) = \frac{\psi(x, \mu) + \psi(x, -\mu)}{2} \quad (2.2)$$

and the odd-parity angular flux as

$$\psi^-(x, \mu) = \frac{\psi(x, \mu) - \psi(x, -\mu)}{2}. \quad (2.3)$$

Combining these three equations and cancelling out the odd-parity component results in

$$-\mu \frac{\partial}{\partial x} \frac{\mu}{\sigma(x)} \frac{\partial}{\partial x} \psi^+(x, \mu) + \sigma(x) \psi^+(x, \mu) = \frac{q(x)}{\sqrt{2}}, \quad (2.4)$$

the one dimensional form of the even-parity neutron transport equation with isotropic scatter. It is an equation in terms of only the even-parity component of the angular flux and has a second-order elliptic diffusion operator. One of the advantages of this form of the neutron

transport equation is the reduction in the number of unknowns, effectively the equation only needs to be solved over half of the angular domain. A result of the elliptic form of the diffusion operator is that spatial discretisations can be obtained which lead to symmetric positive definite matrices. One downside is that there is now a term of the form $1/\sigma$, which will become very large when σ is small, such as in a rarefied gas.

2.2.1 Angular Discretisation

The Legendre polynomials are traditionally used to discretise the angular variable in the slab geometry neutron transport equation. The derivation involves the projection of the equation onto the complete set of basis functions $p_n(\mu)$ for $n = 0, 1, \dots, \infty$. This yields a coupling matrix, between the angular moments, that is non-symmetric due to the use of basis functions which are not orthonormal⁴⁴.

If an angular basis of normalised Legendre polynomials is used, defined in appendix A, the resulting coupling matrix is symmetric. This property is useful later and any further reference to the Legendre polynomials should be taken to mean the normalised version. The even-parity component of the Legendre polynomial basis consists of the set of even moments. The angular basis used for the even-parity equation is then

$$P = \{p_n(\mu) : n = 0, 2, 4, \dots, \infty\}. \quad (2.5)$$

The angular flux can be expanded as a linear combination of this basis using

$$\psi^+(x, \mu) \equiv \sum_{n=0}^{\infty} \psi_{2n}(x) p_{2n}(\mu) \equiv \boldsymbol{\psi}^T(x) \mathbf{p}(\mu) \equiv \mathbf{p}^T(\mu) \boldsymbol{\psi}(x) \quad (2.6)$$

where

$$\boldsymbol{\psi}(x) = (\psi_0(x), \psi_2(x), \dots, \psi_\infty(x))^T, \quad (2.7)$$

$$\boldsymbol{p}(\mu) = (p_0(\mu), p_2(\mu), \dots, p_\infty(\mu))^T, \quad (2.8)$$

and

$$\psi_n(x) = \int_{-1}^1 d\mu p_n(\mu) \psi^+(x, \mu). \quad (2.9)$$

This expansion can now be substituted into eq. (2.4). In order to project the even-parity equation onto the basis the resulting expression must be operated on by $\int_{-1}^1 d\mu \boldsymbol{p}(\mu)$ giving

$$\left[-\boldsymbol{A} \frac{\partial}{\partial x} \frac{1}{\sigma(x)} \frac{\partial}{\partial x} + \sigma(x) \boldsymbol{I} \right] \boldsymbol{\psi}(x) = \boldsymbol{q}(x), \quad (2.10)$$

where

$$\boldsymbol{A} = \int_{-1}^1 d\mu \boldsymbol{p}(\mu) \mu^2 \boldsymbol{p}^T(\mu), \quad (2.11)$$

$$\boldsymbol{I} = \int_{-1}^1 d\mu \boldsymbol{p}(\mu) \boldsymbol{p}^T(\mu), \quad (2.12)$$

$$\boldsymbol{q}(x) = (q(x), 0, \dots, 0)^T \quad (2.13)$$

and the factor of $1/\sqrt{2}$ on the source term has been removed due to the orthogonality of the Legendre polynomials.

The discretised set of equations is in the form of a system of coupled diffusion equations. The coupling is contained in the matrix $\boldsymbol{A}$ which is tri-diagonal and symmetric positive definite.

The first few entries of $\mathbf{A}$ are given below:

$$\begin{pmatrix} \frac{1}{3} & \frac{2}{3\sqrt{5}} & 0 & 0 \\ \frac{2}{3\sqrt{5}} & \frac{3^2}{35} + \frac{2^2}{15} & \frac{4}{7\sqrt{5}} & 0 \\ 0 & \frac{4}{7\sqrt{5}} & \frac{5^2}{99} + \frac{4^2}{63} & \ddots \\ 0 & 0 & \ddots & \ddots \end{pmatrix}. \quad (2.14)$$

The symmetry of this matrix is due to the use of the normalised Legendre polynomials.

Further consideration needs to be given to the isotropic source term $q(x)$. This term contains all fission and scattering sources and has the following multi-group form:

$$q_g(x) = \sum_{g'=1}^G \sigma_{gg'}(x) \psi_{g'0}(x) + \chi_g \sum_{g'=1}^G \nu_{g'} \sigma_{fg'}(x) \psi_{g'0}(x), \quad (2.15)$$

where $q_g(x)$ is the isotropic source in energy group g , the isotropic scattering cross-sections from group g' to group g are represented by $\sigma_{gg'}(x)$, the normalised scalar flux in group g is given by $\psi_{g0}(x)$, the spectrum by χ_g , neutrons released per fission ν and the fission cross-section in group g by $\sigma_{fg}(x)$. If anisotropic scatter was to be included then the use of the normalised Legendre polynomials would require renormalisation of the cross-sections.

So far no approximation, other than isotropy, has been made. The system of equations is infinite in extent and in order to form a closed problem the expansion must be truncated. In order to do this it is assumed that:

$$\psi_n \approx 0 \quad \forall \quad n > N, \quad (2.16)$$

where the odd integer N is the truncation order corresponding to the SP_N equations. In other words an SP_3 expansion includes 2 even moments, ψ_0 and ψ_2 . Odd-order expansions where

N is odd are chosen because it has been found that they are more accurate than even-order expansions⁴⁵.

2.2.2 Transformation into Multi-Group Neutron Diffusion Form

The even-parity SP_N equations in slab geometry have all of the coupling contained in the matrix $\mathbf{A}$ on the diffusion term. Previous applications of a nodal method to the SP_3 equations utilise a simple change of variables to remove this coupling from the diffusion term^{12,16,31,33,35,46}. This process is not explained in general and in this thesis a general transformation of variables is proposed which allows the removal of the coupling on the diffusion term. This will be termed the algebraic diagonalisation. It allows a nodal method to be applied to the SP_N equations in general.

Further to this there is another choice of method to remove the coupling from the diffusion term. A similarity transformation can be defined for the matrix $\mathbf{A}$ which allows the system of equations to be diagonalised³⁸. This process removes the coupling from the diffusion term and, as in the algebraic method, transfers it to the absorption and scatter terms. Both are presented in this section.

Algebraic Diagonalisation of the Angular Coupling Matrix $\mathbf{A}$

The angular coupling matrix $\mathbf{A}$ can be decomposed into two matrices

$$\mathbf{A} = \mathbf{A}_e \mathbf{A}_o \tag{2.17}$$

where o and e denote quantities relevant to the odd and even moments respectively and

$$(\mathbf{A}_e)_{i,i} = \frac{2i-1}{(4i-1)^{1/2}(4i-3)^{1/2}}, \quad (2.18)$$

$$(\mathbf{A}_e)_{i,i-1} = \frac{2(i-1)}{(4i-3)^{1/2}(4i-5)^{1/2}}, \quad (2.19)$$

$$\text{for } i = 1, 2, \dots, \frac{N+1}{2}, \quad (2.20)$$

where $\mathbf{A}_e = \mathbf{A}_o^T$. This is in fact a Cholesky decomposition of $\mathbf{A}$.

The next step is to shift the coupling away from the derivative term yielding a system of coupled diffusion equations analogous to the multi-group diffusion equations. Starting with

$$\left[-\mathbf{A}_e \mathbf{A}_o \frac{\partial}{\partial x} \frac{1}{\sigma(x)} \frac{\partial}{\partial x} + \sigma(x) \mathbf{I} \right] \boldsymbol{\psi}(x) = \mathbf{q}(x), \quad (2.21)$$

a new set of variables is defined

$$\boldsymbol{\phi} = \mathbf{A}_o \boldsymbol{\psi}. \quad (2.22)$$

Substituting this into eq. (2.21) and pre-multiplying by $\mathbf{A}_e^{-1}$ yields

$$-\mathbf{I} \frac{\partial}{\partial x} \frac{1}{\sigma(x)} \frac{\partial}{\partial x} \boldsymbol{\phi}(x) + \mathbf{A}_e^{-1} \sigma(x) \mathbf{A}_o^{-1} \boldsymbol{\phi} = \mathbf{A}_e^{-1} \mathbf{q}(x). \quad (2.23)$$

The right hand side of this equation is a source term and the coupling is contained in the matrix $\mathbf{A}_e^{-1} \mathbf{A}_o^{-1}$ which is symmetric positive definite. This can be proved by considering the expression

$$\mathbf{I} = \mathbf{A}_e \mathbf{A}_e^{-1}. \quad (2.24)$$

Taking the transpose of both sides and utilising $\mathbf{A}_o = \mathbf{A}_e^T$ results in

$$\mathbf{I} = (\mathbf{A}_e^{-1})^T \mathbf{A}_o \quad (2.25)$$

which when right multiplied by $\mathbf{A}_o^{-1}$ yields

$$\mathbf{A}_o^{-1} = (\mathbf{A}_e^{-1})^T. \quad (2.26)$$

This can be substituted into the coupling matrix to give

$$\mathbf{A}_e^{-1} \mathbf{A}_o^{-1} = \mathbf{A}_e^{-1} (\mathbf{A}_e^{-1})^T. \quad (2.27)$$

This demonstrates that a Cholesky decomposition exists for the coupling matrix and therefore it is symmetric positive definite. The matrix inverses involved in the diagonalisation of the SP_N equations are actually trivial to perform as the $\mathbf{A}_n$ matrices are either upper or lower triangular bi-diagonal matrices. The inversion procedure only needs to be performed once in advance.

In order to solve eq. (2.23) using a multi-group diffusion code the coupling terms, off-diagonal terms, in the matrix $\mathbf{A}_e^{-1} \sigma(x) \mathbf{A}_o^{-1}$ can be moved to the right hand side (RHS) to form a source term.

Similarity Transformation of the Angular Coupling Matrix A

In order to remove the coupling on the derivative term an eigenvalue decomposition can be performed on the coupling matrix³⁸

$$\mathbf{A} = \mathbf{R}\mathbf{\Lambda}\mathbf{R}^{-1}, \quad (2.28)$$

where $\mathbf{R}$ is a matrix with the columns formed by the $(N + 1)/2$ eigenvectors $\mathbf{r}_n$ and $\mathbf{\Lambda}$ is a diagonal matrix with the eigenvalues λ_n forming the diagonal. As this matrix is symmetric its eigenvalues must be real and it is always diagonalisable.

The decomposition is feasible for very high numbers of moments because there exists an analytical way of obtaining the eigenvectors and eigenvalues⁴⁴, appendix A. The eigenvalues are given by the squares of the Gauss quadrature points of order $N + 1$, the values at which the zeros of the order $N + 1$ Legendre polynomial occur, where N is the odd-order at which the expansion is truncated. This can be written as

$$\lambda_n \in \{\lambda_n = \mu_m^2 : p_{N+1}(\mu_m) = 0\}. \quad (2.29)$$

The eigenvectors are given by the values of Legendre polynomials evaluated at the μ_n

$$\mathbf{r}_n = (p_0(\mu_n), p_2(\mu_n), \dots, p_{N-1}(\mu_n))^T. \quad (2.30)$$

A new variable is defined

$$\mathbf{R}\phi(x) = \psi(x) = \sum_{n=1}^{\frac{N+1}{2}} \phi_n(x) \mathbf{r}_n, \quad (2.31)$$

where

$$\boldsymbol{\phi}(x) = (\phi_1(x), \phi_2(x), \dots, \phi_{\frac{N+1}{2}}(x))^T. \quad (2.32)$$

As can be seen from the definition, the new variable is a linear combination of the eigenvectors of the matrix $\mathbf{A}$. Substituting the new variable into eq. (2.10) and pre-multiplying by $\mathbf{R}^{-1}$ yields:

$$\left[-\mathbf{R}^{-1} \mathbf{A} \mathbf{R} \frac{\partial}{\partial x} \frac{1}{\sigma(x)} \frac{\partial}{\partial x} + \sigma(x) \mathbf{I} \right] \boldsymbol{\phi}(x) = \mathbf{R}^{-1} \mathbf{q}(x), \quad (2.33)$$

simplifying to

$$\left[-\boldsymbol{\Lambda} \frac{\partial}{\partial x} \frac{1}{\sigma(x)} \frac{\partial}{\partial x} + \sigma(x) \mathbf{I} \right] \boldsymbol{\phi}(x) = \mathbf{R}^{-1} \mathbf{q}(x). \quad (2.34)$$

It is interesting to note that the above derivation very closely follows the proof of equivalence between the slab geometry P_N and S_N equations⁴⁷. It is in fact the even-parity analogue of that proof. Although it is fairly simple to compute $\mathbf{R}^{-1}$ from $\mathbf{R}$ it can actually be done without explicitly computing the inverse. If a diagonal matrix $\mathbf{T}$ is defined which normalises the eigenvectors in $\mathbf{R}$ giving $\mathbf{G} = \mathbf{R} \mathbf{T}$. Now that the eigenvectors are orthonormal $\mathbf{G}^{-1} \equiv \mathbf{G}^T$. This allows us to conclude that $\mathbf{R}^{-1} = \mathbf{T} \mathbf{T}^T \mathbf{R}^T$.

The coupling has been shifted to the term $\mathbf{q}(x)$ which must now be considered in full. The explicit source term is written as

$$\mathbf{q}_g(x) = \sum_{g'=1}^G \sigma_{gg'}(x) \boldsymbol{\psi}_{g'\mathbf{0}}(x) + \chi_g \sum_{g'=1}^G \nu \sigma_{fg'}(x) \boldsymbol{\psi}_{g'\mathbf{0}}(x), \quad (2.35)$$

where $\boldsymbol{\psi}_{g\mathbf{0}}(x) = (\psi_{g0}, 0, \dots, 0)^T$ is a vector containing only the scalar flux. Using eq. (2.31) this scalar flux vector can be transformed into the new space using

$$\boldsymbol{\psi}_{g\mathbf{0}}(x) = \mathbf{R}_{\mathbf{0}} \boldsymbol{\phi}_g(x), \quad (2.36)$$

where $\mathbf{R}_0$ is a matrix containing only the first row of $\mathbf{R}$. This yields a source term of

$$\mathbf{q}_g(x) = \sum_{g'=1}^G \sigma_{gg'}(x) \mathbf{R}_0 \phi_{g'}(x) + \chi_g \sum_{g'=1}^G \nu \sigma_{fg'}(x) \mathbf{R}_0 \phi_{g'}(x). \quad (2.37)$$

It represents a sum not only over the energy groups but also over the ϕ_n to construct the source term. In effect a multi-group problem that initially had G equations, one for each energy group, has been extended to a multi-group problem with $G(N+1)/2$ equations. The set of equations forming this multi-group problem are equivalent to the A_N equations³⁸.

There is one more property of the source term that arises from the similarity transformation that is useful when analysing the performance of the method. The full source term is constructed from matrices that have the form $\mathbf{R}^{-1} \mathbf{R}_0$. Using previous results it can be shown that

$$\mathbf{R}^{-1} \mathbf{R}_0 = \mathbf{T} \mathbf{T}^T \mathbf{R}^T \mathbf{R}_0. \quad (2.38)$$

The matrix $\mathbf{R}^T \mathbf{R}_0$, due to the sparsity of $\mathbf{R}_0$, can be written as $\mathbf{R}_0^T \mathbf{R}_0$ and is therefore positive. Further, $\mathbf{T} \mathbf{T}^T$ is also positive allowing us to conclude that $\mathbf{R}^{-1} \mathbf{R}_0$ is a positive matrix. This means that the augmented group-moment scatter matrix produced in this diagonalisation procedure has only positive entries, exactly as in the multi-group diffusion scatter matrix. This means that all of the analysis done for the multi-group diffusion equations is also valid for this set of equations. This is not true for the algebraic diagonalisation which has negative entries in the group-moment scatter matrix.

To extend this treatment to full Cartesian coordinates, and in doing so form the SP_N equations, the derivatives with respect to x must be replaced with ∇ . This gives

$$\left[- \left(\nabla \cdot \frac{1}{\sigma} \nabla \right) \Lambda + \sigma I \right] \phi = \mathbf{R}^{-1} \mathbf{q}. \quad (2.39)$$

2.2.3 Summary of the Diagonalisation Process

What have been presented above are two methods to remove the angular coupling from the differential term with respect to space and move it onto the source and removal terms. This allows a block Gauss-Seidel method to be applied to solve the coupling between the moments in exactly the same way as a multi-group diffusion solver. It is in fact possible to just take the material data for a model with G groups and expand it into a set of data in $G(N+1)/2$ groups where N is the truncation order. This set of expanded data can in theory be used in a traditional multi-group diffusion solver to obtain a solution to the SP_N equations.

To clarify what is happening the multi-group diffusion equation is presented in a semi-graphical matrix equation form,

$$- \begin{pmatrix} \bullet & & \\ & \bullet & \\ & & \bullet \end{pmatrix} \frac{\partial^2}{\partial x^2} \phi + \begin{pmatrix} \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet \end{pmatrix} \phi = 0 \quad (2.40)$$

where the $\bullet$ represents an entry in the matrix and all others are zero. The SP_N equations can be written in the same form,

$$- \begin{pmatrix} \bullet & \odot & & & \\ \odot & \odot & & & \\ & & \bullet & \odot & \\ & & \odot & \odot & \\ & & & \bullet & \odot \\ & & & \odot & \odot \end{pmatrix} \frac{\partial^2}{\partial x^2} \phi + \begin{pmatrix} \bullet & & \bullet & & \bullet \\ & \odot & & & \\ \bullet & & \bullet & & \bullet \\ & & & \odot & \\ \bullet & & \bullet & & \bullet \\ & & & & \odot \end{pmatrix} \phi = 0 \quad (2.41)$$

where the $\odot$ represents an additional non-zero entry from the angular coupling. It can be observed that the matrix system is now of size $G \times (N+1)/2$.

Performing either of the diagonalisation methods yields the following system of equations,

$$- \begin{pmatrix} \bullet & & & & \\ & \bullet & & & \\ & & \bullet & & \\ & & & \bullet & \\ & & & & \bullet \end{pmatrix} \frac{\partial^2}{\partial x^2} \phi + \begin{pmatrix} \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet & \bullet & \bullet \end{pmatrix} \phi = 0 \quad (2.42)$$

where the $\bullet$ are now any non-zero entry. This system is defined in a fairly arbitrary space but has the form of an extended multi-group diffusion problem. This is what allows one to use the current multi-group nodal diffusion solvers to resolve this system of equations.

2.3 Boundary Conditions

The simplest boundary condition to implement is the reflective boundary condition given by

$$\mathbf{n} \cdot \nabla \phi = 0, \quad (2.43)$$

where $\mathbf{n}$ is the unit outer normal³⁷ and ϕ is defined in eq. (2.31). To the author's knowledge there has been no implementation of a vacuum boundary condition for the SP_N nodal methods in the literature. This is because the applications are mostly infinite lattice, colorset or whole core geometry calculations. In these situations a simple reflective or periodic boundary condition suffices. There are some cases, however, where a vacuum boundary condition may be of some use. For example in a small experimental core where there are large leakages. These are commonly used as validation of the ability of a code to predict pin powers.

The SP_N vacuum boundary conditions have been derived in a number of ways including a variational analysis³ and through equivalence to other forms of the SP_N equations, such as the A_N equations³⁸. In this thesis we will take a more pragmatic approach for nodal methods. The restrictions on the geometry that can be represented by a nodal method result in planar boundaries. This means that on the boundary any given problem reduces to pseudo 1D⁹. It can be expected that the angular variation in the neutron current is roughly the same as in a slab geometry. This means that it is reasonable that a slab geometry neutron transport vacuum boundary condition can be applied to the SP_N equations.

It is not possible to impose the exact vacuum boundary condition and two approximations are commonly used. The first is the Mark boundary condition which corresponds to setting the incoming neutron flux to zero along specific directions which relate to the Gauss quadrature points in 1D. This condition is generally the easiest to impose and is most commonly used. Another, generally more accurate⁴⁷, approximation is the Marshak boundary condition. This involves a moment weighting of the vacuum boundary condition with the odd Legendre polynomials in slab geometry. The moment weighting guarantees that the incoming neutron current is zero. Both will be presented below.

2.3.1 The Mark Boundary Condition

The general vacuum boundary condition in slab geometry is

$$\mu \frac{\partial}{\partial x} \psi^+(x, \mu) \pm \sigma(x) \psi^+(x, \mu) = 0, \quad x \in \Gamma_{\mp}, \quad \mu \gtrless 0, \quad (2.44)$$

for the even-parity flux, where $\Gamma_{\mp}$ represents the left and right boundary points respectively.

The Mark conditions are generated by forcing the incoming angular flux to be zero in the

directions μ_n which correspond to $p_{N+1}(\mu_n) = 0$ where N is the truncation order of the SP_N equations. Substituting in the angular expansion from eq. (2.6) and choosing a particular direction results in

$$\mu_n \frac{\partial}{\partial x} \sum_{\substack{l=0 \\ l \in \text{even}}}^{\infty} \psi_l(x) p_l(\mu_n) \pm \sigma(x) \sum_{\substack{l=0 \\ l \in \text{even}}}^{\infty} \psi_l(x) p_l(\mu_n) = 0. \quad (2.45)$$

Converting this expression to vector notation gives us

$$\mu_n \frac{\partial}{\partial x} \mathbf{p}_n^T \boldsymbol{\psi} \pm \sigma(x) \mathbf{p}_n^T \boldsymbol{\psi} = 0, \quad (2.46)$$

where

$$\mathbf{p}_n = [p_0(\mu_n), p_2(\mu_n), \dots, p_{N-1}(\mu_n)]^T, \quad (2.47)$$

$$\boldsymbol{\psi} = [\psi_0(x), \psi_2(x), \dots, \psi_{N-1}(x)]^T. \quad (2.48)$$

There are $(N+1)/2$ such angles along which this condition must be enforced at each boundary.

Writing them all at once in a matrix equation gives

$$\sqrt{\Lambda} \frac{\partial}{\partial x} \mathbf{R}^T \boldsymbol{\psi} \pm \sigma(x) \mathbf{R}^T \boldsymbol{\psi} = 0, \quad (2.49)$$

where the symbols are defined as per section 2.2.2. The transformation $\boldsymbol{\psi} = \mathbf{R}\boldsymbol{\phi}$ can also be used to give

$$\sqrt{\Lambda} \frac{\partial}{\partial x} \boldsymbol{\phi} \pm \sigma(x) \boldsymbol{\phi} = 0. \quad (2.50)$$

The boundary condition in this form can be applied directly to the transformed equations to approximate a vacuum boundary. This has opened up the possibility of having a vacuum

boundary condition applied to a nodal SP_N code.

The form of the Mark boundary condition presented above is equivalent to that derived for the A_N equations. It is mentioned, in the paper by Ciolini et al.³⁸, that the Mark condition was found to give more accurate solutions than the Marshak condition. This is an unexpected result and the reasons are analysed in the following section.

2.3.2 The Marshak Boundary Condition

The even-parity form of the Marshak condition can be written as

$$\int_{\mu \geq 0} p_m(\mu) \left[\mu \frac{\partial}{\partial x} \psi^+(x, \mu) \pm \sigma(x) \psi^+(x, \mu) \right] d\mu = 0, \quad x \in \Gamma_{\mp}, \quad m \text{ is odd.} \quad (2.51)$$

To simplify the following derivation only the left boundary will be considered, i.e. the half-range integral over $\mu = [0, 1]$. If the right boundary condition is required it can be derived using the same analysis given below due to the symmetry of the Legendre polynomials. The left boundary condition is

$$\int_0^1 p_m(\mu) \left[\mu \frac{\partial}{\partial x} \psi^+(x, \mu) + \sigma(x) \psi^+(x, \mu) \right] d\mu = 0, \quad x \in \Gamma_-, \quad m \text{ is odd.} \quad (2.52)$$

This condition effectively sets the net number of incoming neutrons to zero. Due to this property the Marshak conditions generally introduces less error⁴⁷.

Expanding out the angular variable using eq. (2.6) gives

$$\int_0^1 p_m(\mu) \left[\mu \frac{\partial}{\partial x} \sum_{\substack{l=0 \\ l \in \text{even}}}^{\infty} \psi_l(x) p_l(\mu) + \sigma(x) \sum_{\substack{l=0 \\ l \in \text{even}}}^{\infty} \psi_l(x) p_l(\mu) \right] d\mu = 0. \quad (2.53)$$

In order to proceed further we need to use the half-range integrals over the products of normalised Legendre polynomials. These are modified from Byerly⁴⁸,

$$\int_0^1 p_m(\mu)p_l(\mu)d\mu = \begin{cases} \frac{1}{2} & m = l, \\ 0 & m - l = \text{even}, m \neq l, \\ g_{ml} & m = \text{even}, l = \text{odd}, \\ g_{lm} & m = \text{odd}, l = \text{even}, \end{cases} \quad (2.54)$$

where

$$g_{ml} = \sqrt{\frac{2}{2m+1}} \sqrt{\frac{2}{2l+1}} \frac{(-1)^{(m+l+1)/2} m! l!}{2^{m+l-1} (m-l)(m+l+1) \left[\left(\frac{1}{2} m \right)! \right]^2 \left\{ \left[\frac{1}{2} (l-1) \right]! \right\}^2} \quad (2.55)$$

Starting with the second term in eq. (2.53) we need to evaluate

$$\int_0^1 p_m(\mu) \left[\sigma(x) \sum_{\substack{l=0 \\ l \in \text{even}}}^{\infty} \psi_l(x) p_l(\mu) \right] d\mu = \mathbf{G} \boldsymbol{\psi}, \quad (2.56)$$

where $(\mathbf{G})_{(m/2+1)(l/2+1)} = g_{lm}$ and $\boldsymbol{\psi}$ is defined according to eq. (2.7). The coupling matrix $\mathbf{G}$ is a full matrix coupling all of the even angular expansion coefficients.

The first term omitting the differential operator is

$$\int_0^1 p_m(\mu) \left[\mu \sum_{\substack{l=0 \\ l \in \text{even}}}^{\infty} \psi_l(x) p_l(\mu) \right] d\mu. \quad (2.57)$$

To compute the integrals the recurrence relationship between the Legendre polynomials is

needed. This is given explicitly in appendix A and can be written in the simpler form

$$\mu p_l(\mu) = a_l p_{l+1}(\mu) + b_l p_{l-1}(\mu). \quad (2.58)$$

Using this the first term can be written as

$$\sum_{\substack{l=0 \\ l=\text{even}}}^{\infty} \left[a_l \int_0^1 p_m(\mu) p_{l+1}(\mu) d\mu + b_l \int_0^1 p_m(\mu) p_{l-1}(\mu) d\mu \right] \psi_l(x) \quad (2.59)$$

which after evaluation of the half-range integrals gives

$$\frac{a_{m-1}}{2} \psi_{m-1}(x) + \frac{b_{m+1}}{2} \psi_{m+1}(x) = \mathbf{A}_o \psi, \quad (2.60)$$

with $\mathbf{A}_o$ defined as in section 2.2.2.

Combining the two terms the full Marshak boundary condition in the physical space is

$$\mathbf{A}_o \frac{\partial}{\partial x} \psi + 2\sigma(x) \mathbf{G} \psi = 0. \quad (2.61)$$

This can now be transformed into the abstract space and operated on by $\mathbf{R}^{-1} \mathbf{A}_e$ to give

$$\mathbf{\Lambda} \frac{\partial}{\partial x} \phi + 2\sigma(x) \mathbf{R}^{-1} \mathbf{A}_e \mathbf{G} \mathbf{R} \phi = 0. \quad (2.62)$$

Unlike the approximate Marshak condition presented in the literature³⁸

$$\mathbf{\Lambda} \frac{\partial}{\partial x} \phi + \sigma(x) \phi = 0. \quad (2.63)$$

the boundary condition in eq. (2.62) is coupled between the moments by the matrix $\mathbf{R}^{-1} \mathbf{A}_e \mathbf{G} \mathbf{R}$.

This seems to be the more complete form of the Marshak condition and highlights that eq. (2.63) is an approximation to the Marshak condition. This may go some way to explain why it was found that the Mark boundary condition was more accurate than the Marshak condition³⁸, contrary to previous experience.

2.4 Summary

The SP_N equations are an asymptotic approximation to the neutron transport equation that have been shown to provide improvements in reactor physics calculations. To this end the SP_N equations have been derived and recast into multi-group diffusion form. This has been done in order that existing robust solver techniques, such as the nodal method, can be used to obtain a solution to this equation set. This goes some way to satisfying the objective to implement an SP_N nodal method in this thesis.

The transformation of the SP_N equations allows a nodal method to be applied because the angular coupling matrix has been moved off the differential term. This means that the transverse integration procedure will result in an easy to solve Ordinary Differential Equation (ODE). In practice, for a given neutron diffusion problem, the number of groups is expanded by a multiple of the number of moments retained in the second-order SP_N equations. Using the relationships outlined in this chapter, augmented cross-section sets are defined in the expanded number of “groups”, and the system of equations is solved using existing multi-group neutron diffusion solvers. This process yields the solution to the higher-order SP_N equations.

Two methods of transforming the coupling matrix $\mathbf{A}$ are presented. The first produces negative cross-sections in the augmented scattering matrix which may be pathological to convergence. The second is a similarity transformation and can be shown to give only positive augmented

cross-sections. This means that all of the analysis initially done on the multi-group neutron diffusion equation and related numerical methods holds true. This is a useful result as it opens up the possibility of any code being easily modified to produce an SP_N solution. It is believed by the author that this thesis represents the first time it has been shown that the augmented cross-sections are positive.

The boundary conditions are also outlined for the transformed SP_N equations. The Marshak conditions are in the form of a group independent Robin condition, which can be easily applied to existing codes that incorporate some kind of albedo boundary condition. However, the Marshak conditions are still coupled between the groups. This represents a boundary condition that most existing codes will not be able to apply. The Marshak conditions presented here should produce better results than those published previously for this form of the SP_N equations. The Marshak condition has not been tested as it is much more complicated to implement and would require considerable changes to existing neutron diffusion solvers.

In the next chapter a nodal method will be described for solving the forms of the SP_N equations derived here. Due to the mathematical properties of the system of equations it is sufficient to utilise a method from the literature with only slight modification. A justification is also made for the particular nodal method chosen.

Chapter 3

Nodal Methods

In the previous chapter the SP_N equations have been mapped into a form that can be solved by a standard multi-group diffusion solver. The purpose of this chapter is to develop the multi-group diffusion solver that will be used to solve this system of equations. Traditionally, finite difference type schemes were used for solving the multi-group neutron diffusion equation. It was found that to converge a homogenised reactor core problem a very large number of mesh points were needed to resolve the spatial variation of the neutron flux⁴⁹. This required more memory than was available and also resulted in long execution times for whole cores.

Nodal methods were created to approximate the solution to homogenised neutron diffusion problems with a much smaller number of mesh points, thereby reducing the amount of memory required and increasing the computational efficiency. The accepted figure is that a nodal method can reduce the number of unknowns by around 100 times compared to a finite difference method⁴⁹. The quantities of interest, approximated by a nodal method, are the cell averaged neutron flux and the currents at the surfaces of the cells. In Pressurised Water Reactor (PWR) analysis these cells are generally Cartesian with cuboid domains which represent a whole fuel assembly.

The most commonly used nodal methods are the analytic, semi-analytic and polynomial expansion. The names relate to the types of basis functions used in the approximation of the solution to the system. For more in-depth numerical analysis of the method the reader can refer to the work done by Hennart⁵⁰ and Moulton⁵¹. In order to analyse the nodal schemes equivalences have been drawn with certain types of Finite Element Method (FEM).

There are many sources of information on the derivation and application of nodal methods which will not be repeated here^{49,51–54}. This chapter begins in section 3.1 with a brief discussion of the different types of nodal methods used in reactor analysis. The difficulties encountered by nodal methods when modelling cores with advanced fuels are outlined in section 3.2. This section also provides the justification for the choice of a particular nodal method to solve the system of equations. In section 3.3 the nodal method is derived in full. It should be noted that this derivation is taken from the literature⁵⁵ and reproduced because it is developed further in this thesis.

3.1 Overview of Nodal Methods

The starting point for deriving a nodal method is the multi-group neutron diffusion equation

$$\nabla \cdot \mathbf{J}_g(\mathbf{r}) + \sigma_{tg}(\mathbf{r})\phi_g(\mathbf{r}) = \sum_{g'=1}^G \sigma_{gg'}(\mathbf{r})\phi_{g'}(\mathbf{r}) + \sum_{g'=1}^G \frac{\chi_{g'}\nu\sigma_{fg'}(\mathbf{r})}{\lambda}\phi_{g'}(\mathbf{r}), \quad (3.1)$$

where

$$\mathbf{J}_g(\mathbf{r}) = -D(\mathbf{r})\nabla\phi_g(\mathbf{r}), \quad (3.2)$$

$\phi_g(\mathbf{r})$ is the scalar flux, the subscript g is a specific energy group and G the total number of energy groups, σ_{tg} the total cross-section, $\sigma_{gg'}$ the scatter cross-section from group g' to group

g , σ_{fg} is the fission cross-section, ν the neutrons released per fission, χ_g the neutron spectrum and λ the reactor eigenvalue.

If the diffusion equation is then integrated over a cell (assembly) S_i , with constant material properties, in 2D then the nodal balance relationship is obtained

$$\bar{J}_g(x_{i+1/2}) - \bar{J}_g(x_{i-1/2}) + \bar{J}_g(y_{j+1/2}) - \bar{J}_g(y_{j-1/2}) + \Sigma_{tg}\bar{\phi}_g = \bar{Q}_g \quad (3.3)$$

where

$$\bar{\phi}_g = \frac{1}{\Delta S_i} \int_{S_i} dS \phi_g(\mathbf{r}), \quad \text{cell average flux;} \quad (3.4)$$

$$\bar{J}_g(u) = \frac{1}{\Delta v} \int_v dv \mathbf{J}_g(u, v), \quad \text{face averaged current;} \quad (3.5)$$

$$\bar{Q}_g = \frac{1}{\Delta S_i} \int_{S_i} dS \left[\sum_{g'=1}^G \sigma_{gg'}(\mathbf{r}) \phi_{g'}(\mathbf{r}) + \sum_{g'=1}^G \frac{\chi_g \nu \sigma_{fg'}(\mathbf{r})}{\lambda} \phi_{g'}(\mathbf{r}) \right], \quad \text{cell average source.} \quad (3.6)$$

The nodal balance equation shows that the cell average flux is a function of the neutron currents on the boundary (leakage) and the sources within the cell. In order to compute the global solution interface conditions are required between the cells. These are continuity of the surface fluxes and currents. In order to solve the global problem relationships between the cell average flux and the surface quantities are needed.

At this point there are multiple choices as to how to get the required relationship. Taylor series expansions can be utilised, and these result in finite difference or volume type schemes. To formulate a nodal method the transverse integration procedure is used. This involves integrating

the multi-group neutron diffusion equation over the directions orthogonal to the one under consideration to yield an Ordinary Differential Equation (ODE) for each spatial direction $u = x, y, z$ in terms of a transverse integrated flux

$$-D_g \frac{d^2}{du^2} \tilde{\phi}_g(u) + \Sigma_{tg} \tilde{\phi}_g(u) = \tilde{Q}_g + L_{vg}(u) \quad (3.7)$$

where

$$\tilde{\phi}_g(u) = \frac{1}{\Delta v_i} \int_{v_i} dv \phi_g(\mathbf{r}), \quad \text{face average flux;} \quad (3.8)$$

$$\tilde{Q}_g(u) = \frac{1}{\Delta v_i} \int_{v_i} dv \sum_{g'=1}^G \sigma_{gg'}(\mathbf{r}) \phi_{g'}(\mathbf{r}) + \sum_{g'=1}^G \frac{\chi_g \nu \sigma_{fg'}(\mathbf{r})}{\lambda} \phi_{g'}(\mathbf{r}), \quad \text{face average source;} \quad (3.9)$$

$$L_{vg}(u) = D_g \frac{\partial}{\partial v} \phi_g(\mathbf{r}) \Big|_{v_{i+1/2}} - D_g \frac{\partial}{\partial v} \phi_g(\mathbf{r}) \Big|_{v_{i-1/2}}, \quad \text{the transverse leakage.} \quad (3.10)$$

In order to solve this second-order ODE the form of $L_{vg}(u)$, the transverse leakage, must be known. The transverse leakage term represents the coupling between orthogonal directions. To compute this the exact solution to the whole problem must be known. This of course is not practical and instead an approximation is made.

It has been found through empirical studies that a quadratic basis is sufficient to capture the shape of the transverse leakage term as it does not vary greatly through the domain. Other options exist to represent the leakage, such as using hyperbolic sine and cosine functions or lower order constant and linear representations, but the quadratic representations appears to be sufficient. It should be noted that this is one of the approximations that limits the accuracy of nodal methods. The other is the continuity of average surface quantities. If these approximations are improved then the nodal solution tends to the exact solution.

Once $\tilde{\phi}_g(u)$, the solution to eq. (3.7), is known it contains undetermined coefficients. The values

for these are obtained by enforcing the preservation of the cell average flux and the interface conditions. This results in coefficients in terms of the cell under consideration and its nearest neighbours. For the analytic nodal method this produces a finite difference like stencil, albeit with different coefficients. The system of linear equations formed by doing this for every cell in turn can be solved to produce a global flux profile over all cells.

This process requires knowledge of the previous iteration's solution to compute the quadratic profile for the transverse leakages. Essentially the equations are solved in each direction in isolation and then transverse leakages, coupling terms, are computed. These form additional sources for the next iteration. This non-linear iteration is performed until convergence.

There are a variety of nodal methods and the main differences between them arise from the method used to solve the system of ODEs in eq. (3.7), and the unknowns that the resulting set of equations are written in terms of. The available options for a solution of the ODEs are:

1. analytic,
2. semi-analytic,
3. polynomial expansion.

All of these methods are currently used in reactor physics codes and have been shown to be accurate in benchmark tests and the analysis of real cores. The differences between the methods will be briefly covered in the next sections.

The explicit unknowns, for which the equation set is solved, can be chosen independently from the method used to solve the ODE. The cell average flux is always an unknown, but additionally surface currents or fluxes can also be unknowns. Historically certain solution methods have been identified with certain unknowns, and this will be highlighted in the text. In reality the association of a method with a particular set of unknowns is artificial and the unified nodal methods have highlighted ways of integrating more than one nodal method by solving them in terms of the same unknowns^{56,57}.

A final point to make is that the nodal method can be seen as an acceleration procedure for the finite difference solution to the same problem. It can be shown that in the fine mesh limit that the nodal methods reduce to the finite difference method.

3.1.1 Analytic Nodal Method

In the Analytic Nodal Method (ANM) the homogeneous and particular solution to the transverse integrated expression, eq. (3.7), is found within a cell^{53,54}. Written in matrix form the equation is

$$\left[\mathbf{D} \frac{d^2}{du^2} + \mathbf{\Sigma} \right] \tilde{\boldsymbol{\phi}} = \mathbf{L}_v \quad (3.11)$$

where

$$\tilde{\boldsymbol{\phi}} = [\phi_1, \phi_2, \dots, \phi_G]^T, \quad (3.12)$$

$$\text{diag}(\mathbf{D}) = -[D_1, D_2, \dots, D_G], \quad (3.13)$$

$$(\mathbf{\Sigma})_{gg'} = \sigma_{tg} \delta_{gg'} - \sigma_{gg'} - \frac{\chi_g \nu \sigma_{fg'}}{\lambda}, \quad (3.14)$$

$$\mathbf{L}_v = [L_{v1}(u), L_{v2}(u), \dots, L_{vG}(u)]^T, \quad (3.15)$$

where $\delta_{gg'}$ is a Kronecker delta. From a previous iteration we know an estimate for λ and $\mathbf{L}_v$ and therefore are in a position to obtain the general solution. Using a similarity transformation the coupled second-order ODEs can be separated into G decoupled ODEs

$$\left[\frac{d^2}{du^2} + \boldsymbol{\lambda} \right] \tilde{\boldsymbol{\psi}} = [\mathbf{T}^{-1} \mathbf{D}^{-1}] \mathbf{L}_v. \quad (3.16)$$

where

$$\mathbf{D}^{-1}\mathbf{\Sigma}\mathbf{T} = \mathbf{T}\mathbf{\lambda}, \quad (3.17)$$

$$\tilde{\phi} = [\mathbf{T}] \tilde{\psi}. \quad (3.18)$$

This procedure results in an expression for the flux in each group, which can be used to determine the coefficients for a 5 point finite difference-like stencil. However, it is only practical for problems involving two energy groups. For more than two groups a numerical method is required to perform the similarity transformation. This would need to be done for every material in the reactor and does not scale well as the number of groups increases. For this reason problems of three or more energy groups generally use different methods, such as the Semi-Analytic Nodal Method (SANM) and Nodal Expansion Method (NEM) explained later.

The advantage of the ANM is a reduction in the number of unknowns and the ability to capture steep flux and current gradients. This allows great accuracy in the final solution with the only approximation being that of the form of the transverse leakage. The reactor eigenvalue is determined using standard iterative methods such as the power iteration, which can be accelerated using techniques such as coarse mesh re-balance, Chebyshev acceleration and Weilandt Shift.

3.1.2 Semi-Analytic Nodal Method

The SANM differs from the ANM in the way it treats the group coupling. Due to the inherent problems in solving the ANM in more than two groups it was decided to move the scattering

and production operator onto the Right Hand Side (RHS) of the transverse integrated equation

$$\left[\mathbf{D} \frac{d^2}{du^2} + \mathbf{\Sigma} \right] \tilde{\phi} = \mathbf{M} \tilde{\phi} + \mathbf{L}_v, \quad (3.19)$$

where

$$\text{diag}(\mathbf{\Sigma}) = [\sigma_{t1} - \sigma_{11}, \sigma_{t2} - \sigma_{22}, \dots, \sigma_{tG} - \sigma_{GG}] \quad (3.20)$$

$$(\mathbf{M})_{gg'} = \sigma_{gg'} - \delta_{gg'} \sigma_{gg'} + \frac{\chi_g \nu \sigma_{fg'}}{\lambda}. \quad (3.21)$$

The whole RHS is then approximated with a quadratic function

$$\left[\mathbf{D} \frac{d^2}{du^2} + \mathbf{\Sigma} \right] \tilde{\phi} = \mathbf{a}_0 + \mathbf{a}_1 u + \mathbf{a}_2 u^2, \quad (3.22)$$

yielding a de-coupled set of equations to which the general solution can be written down. This method can therefore be easily implemented for more than two groups and the within-group equation solutions are of a simpler form than the ANM.

The downside is that extra unknowns have been introduced into the equation set. In order to determine these the equation set is moment weighted and the group coupling is approximated by solving this moment weighted equation set instead of the full set. This process is expanded on in later sections.

In summary there are two further approximations than that of the ANM: the quadratic form of the production and scattering sources and moment weighting of the equations in order to determine the group coupling. Although these seem to be a significant departure from the ANM in practice the hyperbolic functions, contained in the within-group solutions, also allow the capturing of very steep flux gradients. It is also found that the SANM performs almost as

well as the ANM, but can be more easily extended to multi-group problems.

There is also another incarnation of the SANM where the transverse integration procedure is not carried out. It involves within-group expansions of non-separable functions in 2D⁵⁸. These remove the need for a transverse leakage approximation but the source term approximation remains. It also has certain advantages connected to the homogenisation and pin power reconstruction procedures. The corner point values are much more accurately obtained using this method and consistent procedures can be developed. The number of unknowns is increased resulting in a computation penalty, and these methods have not found widespread use.

3.1.3 Polynomial Expansion Nodal Method

This method is also applicable in cases with more than two energy groups. The solution to the transverse integrated equations is approximated by n^{th} -order polynomial expansions and the leakages with the traditional quadratic function. The 1D flux is approximated by

$$\tilde{\phi}_g(u) \approx \bar{\phi} f_0(u) + \sum_{n=1}^N a_{ugn} f_n(u) \quad (3.23)$$

where the polynomial basis functions employed are

$$f_0 \equiv 1, \quad (3.24)$$

$$f_1 \equiv \frac{u}{\Delta u} \equiv \xi, \quad (3.25)$$

$$f_2 \equiv 3\xi^2 - \frac{1}{4}, \quad (3.26)$$

$$f_3 \equiv \xi \left(\xi - \frac{1}{2} \right) \left(\xi + \frac{1}{2} \right), \quad (3.27)$$

$$f_4 \equiv \left(\xi^2 - \frac{1}{20} \right) \left(\xi - \frac{1}{2} \right) \left(\xi + \frac{1}{2} \right). \quad (3.28)$$

In the literature the polynomial order chosen is normally four. The unknowns a_{ugn} are determined by a constraint on each boundary, preservation of the cell average flux and a weighted residual procedure for the remaining two unknowns. This allows the discretised equations to be written in response matrix form

$$\bar{\mathbf{J}}_g^{out} = \mathbf{P}_g + [\mathbf{R}_g] \bar{\mathbf{J}}_g^{in} \quad (3.29)$$

where $\bar{\mathbf{J}}_g^{out}$ and $\bar{\mathbf{J}}_g^{in}$ are vectors of the face averaged currents for all of the surfaces; $\mathbf{P}_g$ is the contribution from the leakage and source terms and $[\mathbf{R}_g]$ is a matrix of the expansion coefficients. Using a connectivity matrix,

$$\bar{\mathbf{J}}_g^{in} \equiv [\mathbf{C}] \bar{\mathbf{J}}_g^{out}, \quad (3.30)$$

which relates the outgoing currents from one surface to the incoming currents to another surface (current continuity). The matrix equation to be solved can then be formed

$$[\mathbf{I} - \mathbf{R}_g \mathbf{C}] \bar{\mathbf{J}}_g^{out} = \mathbf{P}_g. \quad (3.31)$$

Traditionally the unknowns in this formulation are the surface currents. This response matrix form then requires different types of solution strategies as the matrix has a significantly different structure⁴⁷. The advantage of the NEM is that it is easy to extend to multi-group and for a large number of groups it will converge more quickly than the ANM or SANM. The polynomial basis also makes it easier to include spatially varying cross-sections in the formulation. This is useful for modelling burnup and mitigating spectral effects from homogenisation. One of the main disadvantages of the NEM is that its accuracy can be limited due to instabilities seen in

the presence of large flux gradients, which are a result of the use of a polynomial basis.

3.2 Challenges to Nodal Methods Produced by Advanced Fuels

The proposed solver is being developed to solve problems which involve cores loaded with Mixed OXide (MOX) and Uranium OXide (UOX) assemblies. This means that the scalar flux gradients will become very large at the boundaries between the two types of assembly. There is a lot of information in the literature about the best nodal method to apply in this situation.

The first consideration is the number of energy groups used in the assembly, colorset or whole core simulation. The neutron energy spectra in MOX and UOX assemblies differ greatly and two energy groups are insufficient to capture the behaviour on the boundaries. For this reason a nodal method capable of performing multi-group calculations is necessary. Further to this, in the transformed SP_N equations there are additional entries in the group structure that correspond to moments of the angular flux. This will, at the very least, double the number of energy groups.

Several implementations of the ANM have been developed which can handle multi-group calculations^{55,59,60}, but all have been reported to take a significant amount of computational effort. It is the full eigenvalue decomposition of the matrix coupling the different energy groups in every node for every nodal update which requires so much effort.

In order to address the limitations of the ANMs the SANMs were developed. Various formulations have been proposed^{52,55,60-63}, but they all revolve around some approximation to the group coupling and subsequent solution of this simpler form. The accuracy of the solution is

found to be comparable to that of an analytical method, but with less computation.

This has led to the SANM⁵⁵ being adopted to solve the proposed form of the SP_N equations. To further accelerate the convergence of nodal methods the Coarse Mesh Finite Difference (CMFD) method is commonly used. This distinction between a nodal method and CMFD is slightly artificial but helps in understanding how the method works as a whole. The CMFD method solves the whole core diffusion problem using the Finite Difference (FD) method with one unknown per assembly. In order to increase the accuracy of this coarse calculation the coupling coefficients between neighbouring nodes are modified to reproduce neutron currents predicted by a more accurate local calculation. The local method in this thesis is the SANM applied to two nodes at a time to obtain the neutron currents on their common interface. This means that efficient solver techniques can be applied to solve the global FD problem, and the accurate local problems only need to be solved for a very small region. The global and local scales are iterated between until convergence is achieved. A significant reduction in storage, i.e. unknowns, is also realised as the full set of coefficients of the flux expansion need only ever be stored for two nodes at a time.

3.3 Derivation of the Semi-Analytic Nodal Method

In order to obtain a solution to the determining equations in the form derived in section 2.2.2 the SANM was chosen with a CMFD formulation for acceleration. The exact formulation used was that of Fu and Cho⁵⁵. The complete derivation will not be reproduced here, only the results pertinent to this work are given. The notation in the original work will be adhered to for clarity.

The starting point is the transverse integrated multi-group diffusion equation

$$-\frac{d}{du}\phi(u) + \hat{\mathbf{S}}\phi(u) = \mathbf{M}\phi(u) - \mathbf{l}(u) \quad (3.32)$$

where

$$\hat{\mathbf{S}} = \mathbf{D}^{-1}(\mathbf{S}_r), \quad (3.33)$$

and

$$\mathbf{M} = \mathbf{S}_s + \frac{1}{k_{\text{eff}}}\chi\nu\mathbf{S}_f. \quad (3.34)$$

u is in a generalised coordinate system and can take the value x, y or z ; $(\phi(u))_g = \phi_g(u)$ is the vector of the group fluxes; $(\mathbf{S}_r)_{gg} = \Sigma_{rg} = \Sigma_t - \Sigma_{gg}$ is a diagonal matrix containing the removal cross-sections for each group; $\mathbf{S}_s\phi(u)$ is the scattering source; $\frac{1}{k_{\text{eff}}}\chi\nu\mathbf{S}_f\phi(u)$ contains the fission source; $\mathbf{l}(u)$ is the transverse leakage pre-multiplied by $\mathbf{D}^{-1}$; $(\mathbf{D})_{gg} = D_g$ is a diagonal matrix containing the diffusion coefficients for each group.

Provided that the source terms on the RHS of eq. (3.32) are projected onto quadratic Legendre polynomials, the general solution is

$$\phi(u) = \mathbf{a}_0 + u\mathbf{a}_1 + \left(u^2 - \frac{h^2}{3}\right)\mathbf{a}_2 + \left(\sinh \sqrt{\hat{\mathbf{S}}}u\right)\mathbf{a}_3 + \left(\cosh \sqrt{\hat{\mathbf{S}}}u\right)\mathbf{a}_4, \quad (3.35)$$

where the $\mathbf{a}_m$'s are vectors of expansion coefficients to be determined.

At any stage in the iterative process, certain information is available to allow computation of the undetermined coefficients. The first is the k_{eff} and the second are the node averaged fluxes,

$\bar{\phi}$. Requiring the preservation of the node average flux results in

$$\mathbf{a}_0 + \mathbf{B}_0 \mathbf{a}_4 = \bar{\phi}. \quad (3.36)$$

To proceed further the determining equations are moment weighted with the first three Legendre polynomials. This results in

$$\hat{\mathbf{S}} \mathbf{a}_0 - 2\mathbf{a}_2 = \mathbf{M} \bar{\phi} + \mathbf{l}_0 \quad (3.37)$$

$$\mathbf{A} \mathbf{a}_1 = \mathbf{M} \mathbf{B}_1 \mathbf{a}_3 - \mathbf{l}_1 \quad (3.38)$$

$$\mathbf{A} \mathbf{a}_2 = \mathbf{M} \mathbf{B}_2 \mathbf{a}_4 - \mathbf{l}_2 \quad (3.39)$$

where the $\mathbf{l}_n$'s are the Legendre expansion coefficients of $\mathbf{l}(u)$ and the $\mathbf{B}_n$'s are given by

$$\mathbf{B}_0 = \frac{1}{\langle 1, 1 \rangle} \left\langle 1, \cosh \sqrt{\hat{\mathbf{S}}} u \right\rangle \quad (3.40)$$

$$\mathbf{B}_1 = \frac{1}{\langle u, u \rangle} \left\langle u, \sinh \sqrt{\hat{\mathbf{S}}} u \right\rangle \quad (3.41)$$

$$\mathbf{B}_2 = \frac{1}{\langle u^2 - \frac{h^2}{3}, u^2 - \frac{h^2}{3} \rangle} \left\langle u^2 - \frac{h^2}{3}, \cosh \sqrt{\hat{\mathbf{S}}} u \right\rangle \quad (3.42)$$

and the inner product is defined as

$$\langle f(u), g(u) \rangle = \int_{-h}^h f(u) g(u) du, \quad (3.43)$$

where h is the half-width of the node and $\mathbf{A} = \hat{\mathbf{S}} - \mathbf{M}$.

It is possible to determine the values of all of the even $\mathbf{a}_m$'s within a given node using the information derived thus far. Equation (3.36), eq. (3.37) and eq. (3.39) can be re-arranged to give

$$(\mathbf{A}\hat{\mathbf{S}}\mathbf{B}_0 + 2\mathbf{M}\mathbf{B}_2)\mathbf{a}_4 = \mathbf{A}(\mathbf{A}\bar{\boldsymbol{\phi}} - \mathbf{l}_0) + 2\mathbf{l}_2. \quad (3.44)$$

Solving the G by G matrix equation above allows us to compute $\mathbf{a}_4$ and through substitution obtain $\mathbf{a}_0$ and $\mathbf{a}_2$. The only coefficients which now need to be determined are the odd ones.

Surface Current and Flux Relationship

To determine the odd coefficients the following surface flux and current relationships are required

$$\phi_{\pm} = \pm h\mathbf{a}_1 \pm \left(\sinh h\sqrt{\hat{\mathbf{S}}} \right) \mathbf{a}_3 + \mathbf{e}_{\phi}, \quad (3.45)$$

$$\mathbf{J}_{\pm} = -\mathbf{D} \left[\mathbf{a}_1 + \left(\sqrt{\hat{\mathbf{S}}} \cosh h\sqrt{\hat{\mathbf{S}}} \right) \mathbf{a}_3 \right] \pm \mathbf{e}_J, \quad (3.46)$$

where

$$\mathbf{e}_{\phi} = \mathbf{a}_0 + \frac{2}{3}h^2\mathbf{a}_2 + \left(\cosh h\sqrt{\hat{\mathbf{S}}} \right) \mathbf{a}_4, \quad (3.47)$$

$$\mathbf{e}_J = -\mathbf{D} \left[2h\mathbf{a}_2 + \left(\sqrt{\hat{\mathbf{S}}} \sinh h\sqrt{\hat{\mathbf{S}}} \right) \mathbf{a}_4 \right]. \quad (3.48)$$

Equation (3.38) can then be used to write the above expressions in terms of the surface currents and fluxes

$$\phi_{\pm} = \mp \mathbf{C} \left(\mathbf{J}_{\pm} - \hat{\mathbf{J}}_{\pm} \right) + \hat{\phi}_{\pm}, \quad (3.49)$$

where

$$\mathbf{C} = \left(h\hat{\mathbf{A}} + \sinh h\sqrt{\hat{\mathbf{S}}} \right) \left(\hat{\mathbf{A}} + \sqrt{\hat{\mathbf{S}}} \sinh h\sqrt{\hat{\mathbf{S}}} \right)^{-1} \mathbf{D}^{-1} \quad (3.50)$$

$$\hat{\phi}_{\pm} = \mp h\hat{l}_1 + \mathbf{e}_{\phi}, \quad (3.51)$$

$$\hat{j}_{\pm} = \mathbf{D}\hat{l}_1 \pm \mathbf{e}_J, \quad (3.52)$$

$$\hat{\mathbf{A}} = \mathbf{A}^{-1}\mathbf{M}\mathbf{B}_1, \quad (3.53)$$

$$\hat{l}_1 = \mathbf{A}^{-1}l_1. \quad (3.54)$$

The important thing here is that $\mathbf{C}$, $\hat{j}_{\pm}$ and $\hat{\phi}_{\pm}$ can be computed for the specific node under consideration.

In order to finally determine the values of the surface fluxes and currents the two-node problem needs to be solved. Consider two neighbouring nodes, the quantities in the node on the left and right of the shared interface are given the superscripts L and R respectively. The continuity of the surface fluxes and currents on the shared interface are then enforced

$$\phi_+^L = \phi_-^R, \quad (3.55)$$

$$\mathbf{J}_+^L = \mathbf{J}_-^R. \quad (3.56)$$

Eliminating the surface fluxes results in

$$(\mathbf{C}^R + \mathbf{C}^L)\mathbf{J}_+^L = (\mathbf{C}^R\hat{j}_-^R - \hat{\phi}_-^R) + (\mathbf{C}^L\hat{j}_+^L + \hat{\phi}_+^L). \quad (3.57)$$

This matrix system can now be solved to obtain the surface currents $\mathbf{J}_+^L$ on the shared interface.

The coefficients of the full expansion have now been determined and the two-node problem

solved. These currents are commonly used in the CMFD method to update the coupling coefficients and force the currents on the coarse scale to converge to those on the fine scale. The use of a more comprehensive basis and the better approximation of the group coupling are the features of this higher-order model, which are being fed back into the coarse scale.

3.4 Summary

In this chapter the use of a nodal method for the applications in this thesis has been justified. This was done by outlining the available nodal methods and discussing their relative strengths and weaknesses. The SANM has been chosen because: it can capture the steep flux gradients at the interface of MOX and UOX assemblies; it can be easily, and efficiently, extended to multiple energy groups; it has comparable accuracy to the ANM.

The specific SANM⁵⁵ chosen has been derived with the notation used in the reference. This has been done as the expressions are necessary in later work. The nodal method has been formulated for the two-node problem, which uses information from the previous global iteration, to obtain a high-order local flux approximation over two nodes. The utility of this local solution in the global scheme is described in the next chapter. It is worth noting that the only reason that the unmodified SANM can be applied to the SP_N equations is due to the work described in section 2.2.2. If the angular coupling matrix had not been removed from the diffusion term, by either of the transformations, then the transverse integrated ODE would contain derivatives of more than one angular moment. Some of these derivatives would have to be approximated in order to solve the ODE introducing further errors. This is the method employed by Smith³⁶ in the code Quadratic Analytic Nodal Transport Method (QUANTM).

Chapter 4

The Coarse Mesh Finite Difference Method

The Coarse Mesh Finite Difference (CMFD) method is viewed as a way to accelerate nodal methods and reduce storage requirements. The acceleration is achieved by iterating between local higher-order calculations and a whole core Finite Difference (FD) calculation. It is possible to converge the global solution to the same level of accuracy of the nodal method without ever explicitly solving the higher-order problem for the whole core. This results in a significant performance gain compared to using a nodal method to solve for the whole core at once.

In the previous chapter a nodal method was developed which, given the cell average fluxes and reactor eigenvalue, is capable of computing accurate surface currents and fluxes on the interfaces between cells. This is done for every interface in a problem using the current global FD solution as input to the nodal method to determine updated surface quantities. These updated currents and fluxes are then used to define coupling coefficients, in the global FD method, that can reproduce the higher-order local currents. The global problem is then solved with the coupling coefficients and the process repeated.

It is the definition of these coupling coefficients in the global FD calculation that distinguishes each CMFD method. By changing the coupling coefficients, to reflect a higher-order solution, the eigenvalue and fluxes of the global problem will be pushed closer to that of the higher-order solution. Unfortunately there is not much mathematical analysis of this non-linear iteration, but it has been observed in practice to converge in most cases. In some situations the coupling coefficients are changed to the point where they invalidate the assumptions made about the coupling matrix and the solvers are unable to converge. This behaviour is explained later in this chapter.

The definition of the coupling coefficients, used to update the global calculation, has been recently revisited^{64,65} in an effort to define more rigorous and stable expressions. The result was the derivation of consistent coupling coefficients for the multi-group Analytic Nodal Method (ANM) called Effective Diffusion Coefficients (EDCs). It was reasoned that these consistent coupling coefficients should provide additional stability. In this chapter the EDCs for the Semi-Analytic Nodal Method (SANM) are derived following an identical procedure and result in a similar form. To the author's knowledge this is the first time that the EDCs have been derived for this type of nodal method.

In this chapter the CMFD methods will be reviewed in section 4.1. In light of the work done on the EDCs a set will be developed for the SANM in section 4.2. Now that the SP_N equations are derived and a nodal and CMFD combination have been chosen, the specific implementation in the Pwr and Agr Neutronics and Thermal Hydraulics Evaluation Route (PANTHER) code will be outlined in section 4.3.

4.1 Overview of Existing Methods

The starting point for the CMFD method is the FD expression for a cell k of the mono-energetic neutron diffusion equation in slab geometry. This is

$$J_+ - J_- + \sigma_{tk}\bar{\phi}_k = \bar{q}_k, \quad (4.1)$$

where

$$J_- = -D_-(\bar{\phi}_k - \bar{\phi}_{k-1}), \quad (4.2)$$

$$J_+ = -D_+(\bar{\phi}_{k+1} - \bar{\phi}_k), \quad (4.3)$$

and $D_{\pm}$ are harmonic averages of the diffusion coefficients on either side of the right (+) and left (−) interface. It is clear that this expression is just the nodal balance equation with a rough approximation of the currents. Given a source q , if we can get the surface current expressions correct, the cell average flux will be calculated correctly.

The most intuitive method to correct the currents was developed by Smith⁶ (KS) and involved writing the surface currents in a slightly different form

$$J_+ = -D_+(\bar{\phi}_{k+1} - \bar{\phi}_k) + \bar{D}_+(\bar{\phi}_{k+1} + \bar{\phi}_k). \quad (4.4)$$

Here $\bar{D}_+$ is the term used to correct the current.

At any point during the solution procedure the latest cell average fluxes and eigenvalue are known and more accurate currents can be predicted using the nodal method. This means that eq. (4.4) can be used to determine what $\bar{D}_+$ is needed to reproduce the more accurate current.

This value can then be added to the FD matrix so that the next global solution can reflect the local solutions.

Two other methods called the Moon et al.⁷ (MCNH) and Aragoes and Ahnert⁵ (AA) methods have a slightly more involved form of the correction factor. Instead of a single correction factor per interface, $\bar{D}_+$, there are now two correction factors. Allowing the extra degrees of freedom results in the following expression for the surface current

$$J_+ = -(D_{k+1}^- \bar{\phi}_{k+1} - D_k^+ \bar{\phi}_k), \quad (4.5)$$

where $D_k^\pm$ is an expression involving the diffusion coefficients and correction factors for the right (+) and left (−) surfaces of node k .

This process reduces the storage requirements of a nodal code by reducing the number of unknowns. Instead of having to store 5 expansion coefficients to represent the flux for every group in every node, they only ever need to be stored for two nodes at a time while updating the coupling coefficients and can then be discarded. The coupling coefficients then carry the information from the high-order local calculation to the global low-order calculation in a very concise form.

All three of the methods above appear to have been introduced in an *ad hoc* manner with no link to underlying theory. It is important to notice that each method essentially defines a correction factor which modifies a standard FD matrix. The intention is that the largest positive eigenvalue and eigenvector of the CMFD matrix are pushed closer to the whole core higher-order solution. However, each definition of the correction factor results in a different FD matrix, all of which are capable of reproducing the higher-order solution in theory. The difference between the methods lies in the other excited eigenmodes of the FD matrix. This

matters because it will have an impact on the efficiency of the iterative scheme used to solve the corrected FD matrix produced by each method.

Ideally each method should preserve the convergence properties that the FD matrix possesses. This is possible even though symmetry is immediately lost after the first update. Properties such as diagonal dominance are sufficient for the convergence of Jacobi type iterative schemes and these can be preserved during updates, although not in general. For certain problems the higher-order solution can be so different that infinite or negative values are computed for the correction factors making solution either impossible or requiring more sophisticated (expensive) numerical methods, such as the Biconjugate Gradient STABilised (BCGSTAB) method⁶⁶.

Specific Considerations Relating to the SP_N Equations

The KS formulation is adequate for diffusion-like problems as the $\bar{\phi}_k > 0$. This means that when using eq. (4.4) to determine $\bar{D}$ from the higher-order solution, there will be no division by zero. However, if one is solving the algebraic second-order form of the SP_N equations in section 2.2.2, it can be reasonably expected that $\bar{\phi}_{k+1} + \bar{\phi}_k = 0$ and a correction cannot be determined. This has been found to be the case by the author on a Mixed OXide (MOX)-Uranium OXide (UOX) interface.

In fact, all of the *ad hoc* correction factors were found to suffer from this effect. It was less pronounced for the MCNH formulation, but still rendered the CMFD unusable for this form of the SP_N equations. For this reason the EDCs were developed for the SANM to provide a rigorous definition of the CMFD current. The aim is to remove situations where it is impossible to define a correction factor.

When the similarity transformation form of the SP_N equations in section 2.2.2 is used this problem disappears. A result of the cross-sections being positive is that all of the solution fields

are positive and the issues in the convergence of the CMFD are no worse than for diffusion. In fact, it was found that both KS and the MCNH definitions resulted in convergence for all test problems. This seems to also confirm the analysis presented in section 2.2.2. There are still possible performance gains from developing EDCs for the SP_N nodal method and this is done in the next section.

4.2 Effective Diffusion Coefficient for the Semi-Analytic Nodal Method

The full expansion of the transverse integrated neutron flux from the SANM is

$$\phi(u) = \mathbf{a}_0 + u\mathbf{a}_1 + \left(u^2 - \frac{h^2}{3}\right)\mathbf{a}_2 + \left(\sinh \sqrt{\hat{S}}u\right)\mathbf{a}_3 + \left(\cosh \sqrt{\hat{S}}u\right)\mathbf{a}_4. \quad (4.6)$$

The full derivation of the EDCs is given in appendix B and the resulting form of the surface currents is

$$J_{\pm} = \mp \frac{D}{hC^j} (\phi_{\pm} - C^f \bar{\phi} - Q_{\pm}) \quad (4.7)$$

where

$$C^j = \frac{\tanh \sqrt{\hat{S}}h}{\sqrt{\hat{S}}h}, \quad (4.8)$$

$$C^f = \frac{2h\sqrt{\hat{S}}}{\sinh 2h\sqrt{\hat{S}}}, \quad (4.9)$$

$$Q_{\pm} = (1 - C^f)a_0 \pm h(1 - C^j)a_1 + 2h^2(1/3 - C^j)a_2, \quad (4.10)$$

$\phi_{\pm}$ is the surface flux on one of the surfaces and h is the half-width of the cell.

This expression is exact for the interface current and is in terms of the coefficients of the expansion of the within-group flux. These are known for a given interface once the two-node SANM equations have been solved. In order to write them in terms of the quantities in the FD formulation the continuity conditions for an interface are used.

This results in the following expression for the surface current

$$J = -(\bar{D}_{k+1}\bar{\phi}_{k+1} - \bar{D}_k\bar{\phi}_k) \quad (4.11)$$

where

$$\bar{D}_{k+1} = - \left[\frac{h_k C_k^j}{D_k} + \frac{h_{k+1} C_{k+1}^j}{D_{k+1}} \right]^{-1} \left(C_{k+1}^f + \frac{Q_-}{\bar{\phi}_{k+1}} \right) \bar{\phi}_{k+1}, \quad (4.12)$$

$$\bar{D}_k = - \left[\frac{h_k C_k^j}{D_k} + \frac{h_{k+1} C_{k+1}^j}{D_{k+1}} \right]^{-1} \left(C_k^f + \frac{Q_+}{\bar{\phi}_k} \right) \bar{\phi}_k. \quad (4.13)$$

These define the EDCs, $\bar{D}_k$ and $\bar{D}_{k+1}$, in nodes k and $k+1$, replacing the normal harmonic averages, D_k and D_{k+1} , which define the FD approximation to the current.

It further can be shown that⁶⁵

$$\lim_{h \rightarrow 0} -(\bar{D}_{k+1}\bar{\phi}_{k+1} - \bar{D}_k\bar{\phi}_k) = -(D_{k+1}\bar{\phi}_{k+1} - D_k\bar{\phi}_k) \quad (4.14)$$

which is the FD approximation to the current. This is a desirable property and shows that as the node size becomes small then the numerical method reduces to FD. This is part of the reason why nodal methods perform best for large nodes.

Interestingly the definition of the EDCs was extended to allow the definition of the CMFD current with a diffusion model on the coarse scale and a transport model as the local higher-

order method in 1D⁶⁴. The aim was to accelerate the solution of the global transport problem by only computing the transport solution locally and propagating the information globally with the corrected diffusion model. These transport EDCs were not implemented however.

What has been presented here is the first application of an EDC to accelerate the solution of a global transport problem using the framework of CMFD. In this case the name Coarse Mesh Finite Difference is slightly misleading. What has in fact been done is the acceleration of a nodal solution to the SP_N equations using a global finite difference method for the SP_N equations. A slightly different method can also be imagined whereby the global transport solution is accelerated by using a global diffusion model to propagate information and an SP_N nodal method to obtain the local solutions. In order to derive an EDC to allow acceleration of the SP_N using whole core diffusion a strict definition of the current in SP_N is needed. These have been proposed by Sanchez⁹, but not attempted here.

There is one further comment from the standpoint of implementation in a nodal code. Traditionally every time that a nodal update is performed the whole core CMFD iteration matrix must be updated. The idea is that the nodal update will change the CMFD iteration matrix so that the solution tends successively closer to the whole core nodal solution.

With the earlier definitions of the current correction, the impact of the nodal update on the iteration matrix is problem specific. This means that the convergence of the system after a nodal update could be slow or at worst non-existent due to the removal of some desirable properties such as symmetry, diagonal dominance or positive definiteness.

Although it was found that using the EDCs resulted in very little instability, this situation can be circumvented in the SANM to some extent by a simple rearrangement of eq. (4.11). Instead of combining the $Q_{\pm}$ terms into the current relations they are separated out to give

$$J = -(\overline{D}_{k+1}\overline{\phi}_{k+1} - \overline{D}_k\overline{\phi}_k) + \overline{Q} \quad (4.15)$$

where

$$\overline{D}_{k+1} = - \left[\frac{C_k^j}{D_k} + \frac{C_{k+1}^j}{D_{k+1}} \right]^{-1} C_{k+1}^f \overline{\phi}_{k+1}, \quad (4.16)$$

$$\overline{D}_k = - \left[\frac{C_k^j}{D_k} + \frac{C_{k+1}^j}{D_{k+1}} \right]^{-1} C_k^f \overline{\phi}_k, \quad (4.17)$$

$$\overline{Q} = - \left[\frac{C_k^j}{D_k} + \frac{C_{k+1}^j}{D_{k+1}} \right]^{-1} (Q_- - Q_+). \quad (4.18)$$

This effectively removes the division of the source term by the flux seen in eq. (4.12). This division by the flux can lead to convergence problems when the flux is very small or zero.

The re-arrangement proposed above has removed the flux, effectively a non-linearity, from the definition of the EDCs. The EDCs and therefore the iteration matrix of the CMFD can now be defined at the beginning of the calculation and never need to be updated. The iteration matrix also appears to be diagonally dominant, although non-symmetric, guaranteeing convergence using Jacobi methods for many problems. Every time a new nodal update is performed a new $\overline{Q}$ is computed which is added to the source term instead of the FD matrix. This opens the possibility of computing the inverse of the iteration matrix explicitly and storing it at the beginning of the solution procedure.

The convergence of the CMFD method is now dependent only on the assumption that the successive nodal updates move the CMFD solution closer to that of the SANM. It no longer has a dependence on the updates to the iteration matrix, the convergence properties of which can be checked in advance. For these reasons the form of the EDCs given in eq. (4.15) have been implemented in the SP_N nodal method, along with the KS and MCNH definitions.

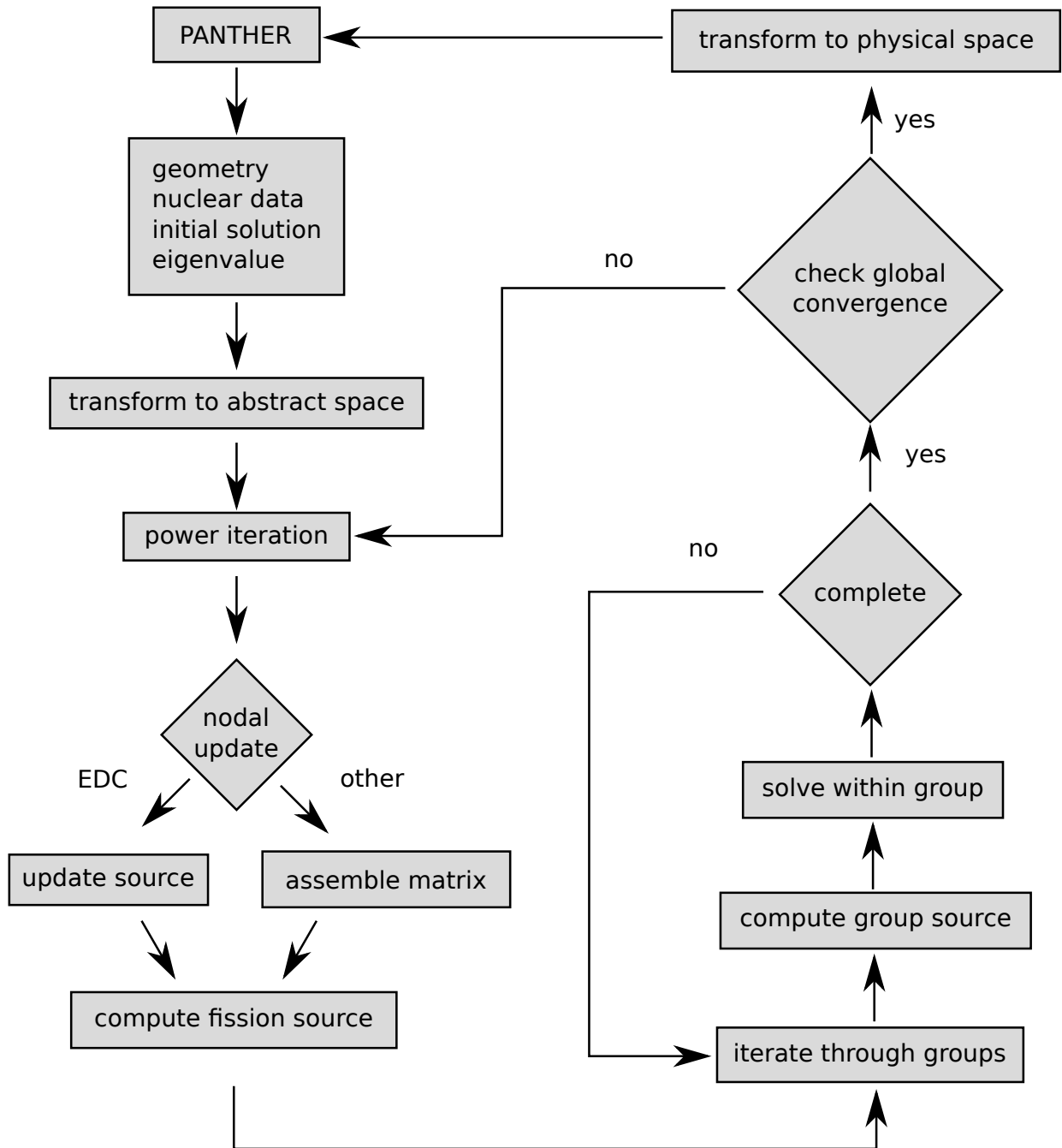
The removal of the non-linearity in the definition of the EDCs can only be done for the SANM as the ANM requires the current eigenvalue to compute the terms in the EDCs and this results in the iteration matrix being modified at each power iteration. As the SANM and ANM results have been found to be close enough for practical purposes^{55,60–62}, the use of the EDCs with the SANM may result in some reduction of computation times and more stable behaviour.

4.3 Implementation of the SP_N Nodal Method

Now that all of the required theory of the nodal SP_N method has been presented information about the implementation can be given. The code has been designed to improve solutions within the PANTHER reactor analysis package. To retain the flexibility needed for research a self-contained solver has been written that can read input from PANTHER. The full geometry and operating conditions of a problem are specified within PANTHER and the internally generated data are then sent to the solver and the solutions returned. Essentially the internal nodal method has been swapped for an external SP_N nodal method. This can then be used in conjunction with more complicated calculational schemes already developed in PANTHER.

A schematic of the external SP_N nodal method is shown in fig. 4.1. The solver needs to be passed the geometry, nuclear data, an initial solution and the eigenvalue. The data is then transformed into the abstract space defined by either the algebraic or similarity method and the power iteration is then commenced.

A nodal update is performed using either the EDCs or the other *ad hoc* methods, although on the first iteration this step is skipped and either an FD or EDC iteration matrix is used with zero transverse leakage assumed. The fission source is then updated and the power iteration continues.

Figure 4.1: Schematic of the SP_N nodal method.

The next step is to iterate through the groups solving each set of within-group equations. This can be done once or until convergence is achieved. The default setting is once as it is found to be more efficient not to converge the group structure totally, as the fission sources are not converged either.

The global convergence of the fluxes and eigenvalue is then checked to terminate the power iteration. If convergence has been reached then the solution is transformed back into the physical space and only the scalar fluxes and surface currents are passed back to PANTHER.

4.3.1 Initial Results

A set of simple test cases was constructed to evaluate the performance of the various CMFD methods with the SP_N equation sets. They included homogeneous 1, 2 and 3D cases in a vacuum with 1 or 2 energy groups. There were also problems with two different materials in contact, one highly absorbing and the other with high production.

These tests were run with both the algebraic and similarity transformation forms of the SP_N equations and all of the implemented CMFD methods: KS, MCNH and EDCs. For the algebraic form of the equations, the KS formulation could not converge to a solution for all cases, and the MCNH did not perform much better. The most interesting result was that the EDCs converged for all simple test cases. A subset of the results for the simple test cases is given in table 4.1 to illustrate this.

It was concluded that for KS and MCNH the definition of the coupling coefficients led to instability of the method. On the interfaces between very different materials, the solution field changes sign and goes through zero. It is possible that on a given interface the flux can be close to zero leading to large numbers in the iteration matrix due to a division by the flux in the

Table 4.1: k_{eff} values from a simple 2D test case involving a checkerboard of 2 different materials. One material is highly fissile and the second highly absorbing. The results are for the SP_3 equations using both the similarity and algebraic transformation. The increasing number of degrees of freedom (DOF) corresponds to refining the mesh. The inability of the solver to converge to a solution was seen when using the algebraic transformation with the KS or MCNH formulations. In contrast to this, the similarity transformation is stable for all formulations.

DOF	Algebraic			Similarity		
	KS	MCNH	EDC	KS	MCNH	EDC
8	0.72572	0.72572	0.72572	0.72425	0.72425	0.72425
32	0.72721	0.72485	0.72485	0.72452	0.72452	0.72452
72	div	0.72502	0.72502	0.72495	0.72495	0.72495
128	div	div	0.72512	0.72510	0.72510	0.72510
200	div	0.72495	0.72518	0.72517	0.72517	0.72517
288	div	0.72521	0.72521	0.72521	0.72521	0.72521
392	0.72523	div	0.72523	0.72523	0.72523	0.72523
512	0.72524	0.72524	0.72524	0.72524	0.72524	0.72524
648	0.72525	0.72525	0.72525	0.72525	0.72525	0.72525
800	0.72526	0.72526	0.72526	0.72526	0.72526	0.72526

definitions of the coupling coefficients. This caused all of the implemented iterative schemes to diverge including BCGSTAB⁶⁶.

For the EDCs the traditional form has a leakage term Q , in eq. (4.12), that is divided by the flux. This makes it susceptible to a similar problem in the presence of near zero fluxes. The modified form gets around this by not dividing by the flux, meaning that convergence can be achieved for a larger class of problems. However, neither achieved convergence for more realistic problems and this rules out the algebraic form of the SP_N equations. What has been highlighted, however, is the superior stability of the EDCs.

For the same set of tests the similarity transformed SP_N equations could be solved by all of the methods. As mentioned before, this is expected as the SP_N equation set retains all of the mathematical properties of the multi-group diffusion equation.

4.4 Summary

In this chapter various CMFD methods have been reviewed for use in combination with the SANM and the SP_N equations. Critically it has been found that the use of the most common forms of the CMFD correction factors mean that some problems will not converge using the algebraic transformation. For this reason the EDCs developed by Chao⁶⁵ were implemented as their use should offer greater stability. This has been observed to be the case by the author, but they still cannot converge the algebraically mapped form of the SP_N equations reliably.

In contrast, when the similarity transformed version of the SP_N equations was used, convergence was achieved in all cases using every CMFD method. This is due to the positivity of all of the cross-sections in the combined group-moment scattering matrix. It was decided that the EDCs would be retained for both forms of the SP_N equations. This is in spite of the fact that they do not appear necessary for the similarity transformation. The reason is that the stability gains observed when testing the algebraic transformation might prove useful for the similarity transformed version of the equations. Furthermore, using the EDC formulation leads to improved computational efficiency and this is quantified fully in the next chapter.

The implementation of the EDCs has been changed slightly from that presented by Chao⁶⁴. In a standard CMFD method at each nodal update new coupling coefficients are computed and the FD matrix recomputed to reflect this. However, a consequence of the SANM being used is that the FD matrix no longer needs to be updated. A correction can be applied to the source term instead and the FD matrix can be computed once and stored. The convergence of this stored FD matrix can then be determined in advance from the nuclear data and geometry. This means that the convergence of the method relies solely on the convergence properties of the non-linear iteration and not on the changes to the iteration matrix produced by the KS,

MCNH and traditional definition of the EDCs. Further, the author believes that this is the first time the EDCs have been used to accelerate the SP_N equations.

The integration of the SP_N nodal method with PANTHER has also been detailed. The SP_N nodal method can import the geometry and nuclear data as specified in PANTHER and after convergence the scalar fluxes, eigenvalue and surface currents can be returned in the appropriate format.

There is only one difference between the SP_N nodal method and a multi-group diffusion nodal method. This is a module that can transform the cross-sections into the abstract space and the solution back to the physical space. If this module is included in any existing multi-group diffusion solver it should be capable of computing a solution to the SP_N equations.

Now that all of the features of the new SP_N nodal solver have been described in detail the necessary benchmarking can be done to test the performance. The next chapter features a set of benchmarks which test all of the aspects of the nodal method covered in the previous chapters.

Chapter 5

Verifying the SP_N Nodal Method

In the previous chapters the theory required to implement an SP_N nodal method has been developed. The final implementation is a Semi-Analytic Nodal Method (SANM) applied to the similarity transformed version of the SP_N equations. This is accelerated using a Coarse Mesh Finite Difference (CMFD) method with the Smith⁶ (KS), Moon et al.⁷ (MCNH) or Effective Diffusion Coefficients (EDCs) as the coupling coefficient definition. The option of using either reflective or Mark vacuum boundary conditions has also been included.

In order to be confident in the performance of the method a comprehensive set of benchmarks have been conducted. These have been selected with a view to testing all of the options in the solver, and the final applications. The first benchmark, in section 5.1, is NEACRP-L-336 which is a pin-by-pin diffusion calculation of various colorset configurations. In section 5.2 a set of homogeneous assembly and pin-by-pin colorset problems prepared by Électricité de France (EDF) are solved. These are designed to test the SP_N solver and have reference solutions from a Finite Element Method (FEM) formulation of the first-order SP_N equations.

The Brantley and Larsen problem in section 5.3 is chosen to highlight the behaviour of the SP_N

equations. It is a quasi 1D problem for which the SP_N equations should be able to provide a good approximation to the P_N equations. The last benchmark, described in section 5.4, is taken from a suite of neutron transport verification test cases originally developed by Takeda and Ikeda⁴. The particular Takeda benchmark test case is a model of a small experimental Light Water Reactor (LWR) core. It is a particularly challenging test case for both the SP_N equations and the nodal method developed in this thesis, which will be discussed in section 5.4. These two test cases have a vacuum boundary condition which allows the implementation of the Mark boundary condition to be fully tested. Finally, these two verification test cases also have full transport reference solutions for comparison.

5.1 NEACRP-L-336

In order to verify that the SP_N nodal method can reproduce the results of previous diffusion nodal methods, the NEACRP-L-336 benchmark⁶⁷ was performed. The chosen cases for comparison are C3, C4 and C5. These are all pin-by-pin models of an array of 2x2 assemblies, each having 17x17 pins. The geometry is shown in fig. 5.1.

The C3 case is an ILC for a Mixed OXide (MOX)-Uranium OXide (UOX) colorset. The C4 case consists of only the assemblies with a zero flux condition applied where the reflector would be. The C5 case has an additional reflector region composed of water and a zero flux boundary condition applied at the edge. The cross-sections for each material are specified in 2 energy groups and the assemblies are either MOX or UOX containing water holes. The MOX assemblies have zoned enrichment where the outermost pincells have a lower enrichment than those in the centre. This is done to reduce the flux gradients at the assembly boundaries.

The presentation of the results here is brief and only the eigenvalues are provided in table 5.1.

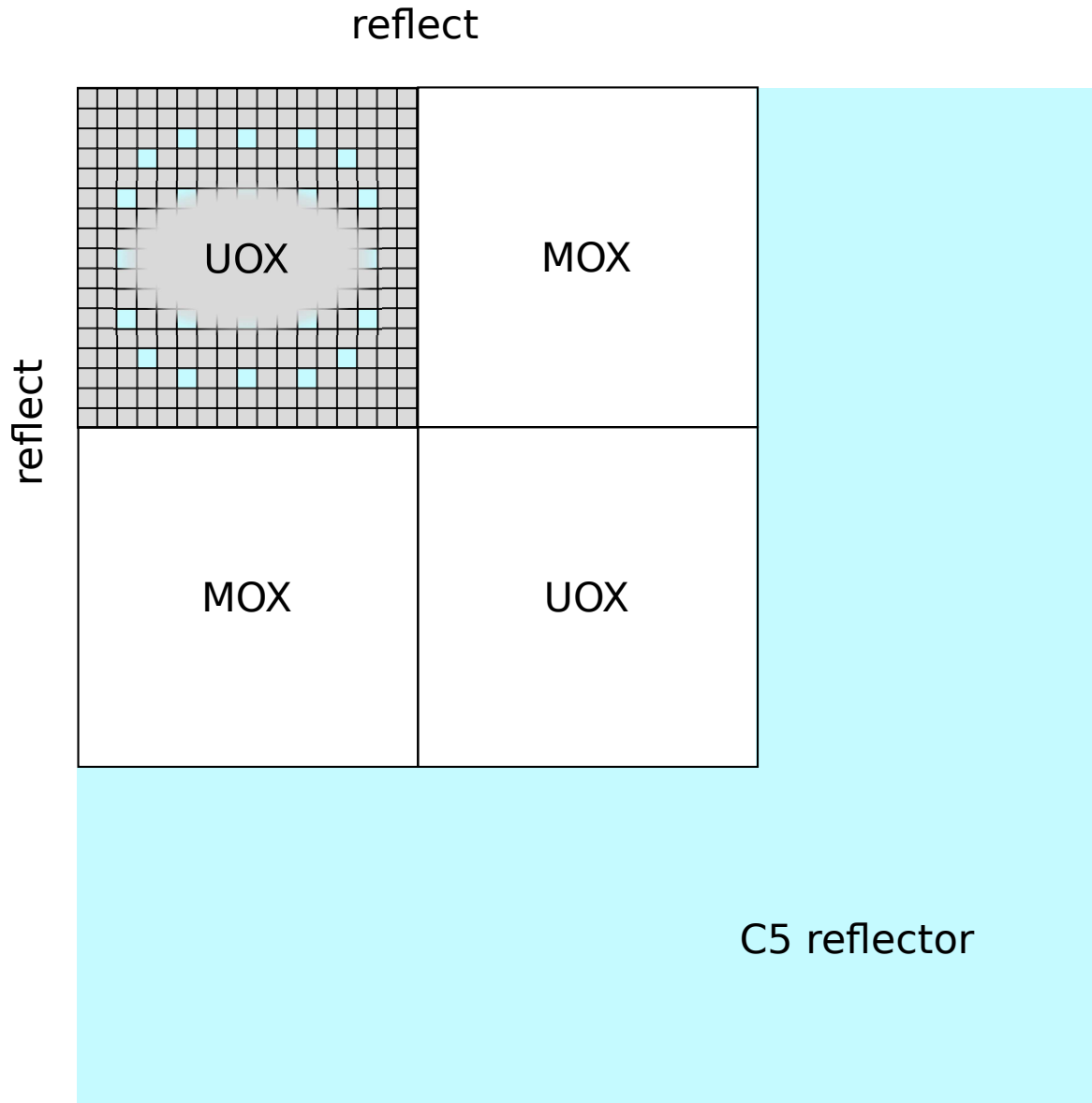


Figure 5.1: The schematic above shows the geometry for the C3, C4 and C5 cases of the NEACRP-L-336 benchmark. The C3 case is an ILC for the colorset without the reflector. The C4 case has a zero flux boundary condition in place of the reflector. The C5 case includes the reflector and has a zero flux boundary at the periphery of the solution domain.

Table 5.1: k_{eff} values for the NEACRP-L-336 benchmark.

Configuration	C3	C4	C5
Benchmark Result (average)	1.01913	0.90677	0.93796
Benchmark Standard Error	0.00005	0.00012	0.00018
SP_N Nodal Method	1.01911	0.90682	0.93804
PANTHER	1.01911	0.90682	0.93804
Fu and Cho ⁵⁵			0.93761

In the original presentation of the SANM⁵⁵ implemented here a result is included for the C5 benchmark which has been included in the table.

It can clearly be seen from the results that the SP_N nodal method is capable of computing highly accurate solutions to diffusion problems. For diffusion problems the multi-group transformation is not performed, and the cross-sections are exactly the same as any other diffusion nodal method. It is found that the solutions from the SANM are almost identical to the Analytic Nodal Method (ANM) in PANTHER. The discrepancy between the value of the C5 k_{eff} from the original paper and this implementation is assumed to be due to insufficient convergence of the solution from the literature.

5.2 EDF Benchmark Suite

The suite of test cases chosen by EDF to verify the SP_N capabilities of their new code COCAGNE all have the same general geometry. It is a grid of 3x3 assemblies each of which have 17x17 fuel pins. The material properties are all derived from APOLLO2 lattice cell calculations and are homogenised into either pin size regions or assembly size regions. This splits the benchmark into two initial categories, heterogeneous and homogeneous assembly models. The number of energy groups explicitly modelled in this benchmark are 2 and 8.

The benchmark suite can test a wide range of the features of COCAGNE and has reference

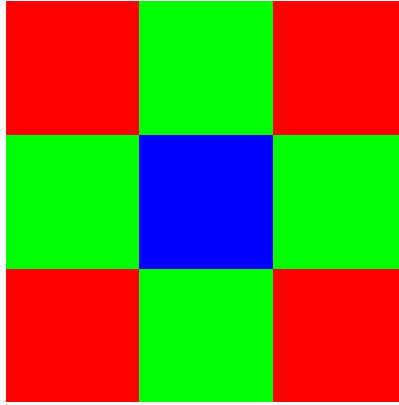


Figure 5.2: The geometry used in the EDF benchmark suite. Each colour represents a different assembly type forming a 3x3 colorset problem which is solved in an infinite lattice calculation. There are both heterogeneous (explicit fuel pins) and homogeneous (one material per assembly) calculations.

transport solutions from APOLLO2 to compare against homogenised SP_N calculations. In this work, the only requirement is to test the precision of the SP_N nodal method and so a simple comparison set was chosen. APOLLO2 was used to generate the material data for a variety of assemblies which were loaded in the configuration shown in fig. 5.2. One problem is a homogeneous core where all assemblies are the same; another has a mixture of assemblies producing relatively small inter-assembly currents; and the third case has a combination of assemblies chosen to produce steep inter-assembly currents. These three cases are felt to represent a wide selection of realistic core conditions while providing a test for all aspects of the numerical method.

5.2.1 Methodology

The reference solutions for all cases are obtained from well converged COCAGNE calculations.

The nodal SP_N solver was used for all combinations of the following benchmark options:

1. flux gradient - flat (single material), moderate, steep;
2. SP_N order - 1, 7;
3. energy groups - 2, 8;
4. geometry - homogeneous (assembly), heterogeneous (pincell).

For the homogeneous calculations there is one set of material properties per assembly sized region. The number of meshes per assembly is refined from the coarsest scale (one mesh per assembly) until the results are converged. For the heterogeneous calculations there is one mesh per pin region, each with the possibility of a distinct set of material properties. No refinement is carried out for the heterogeneous cases as they are expected to be sufficiently converged.

For all cases the k_{eff} is compared to the reference value from EDF. For the heterogeneous cases the fluxes are normalised to unit production to allow for comparison. This is defined as:

$$\sum_{g=1}^G \int_V \nu \sigma_{fg}(\mathbf{r}) \phi_{0g}(\mathbf{r}) dV = 1, \quad (5.1)$$

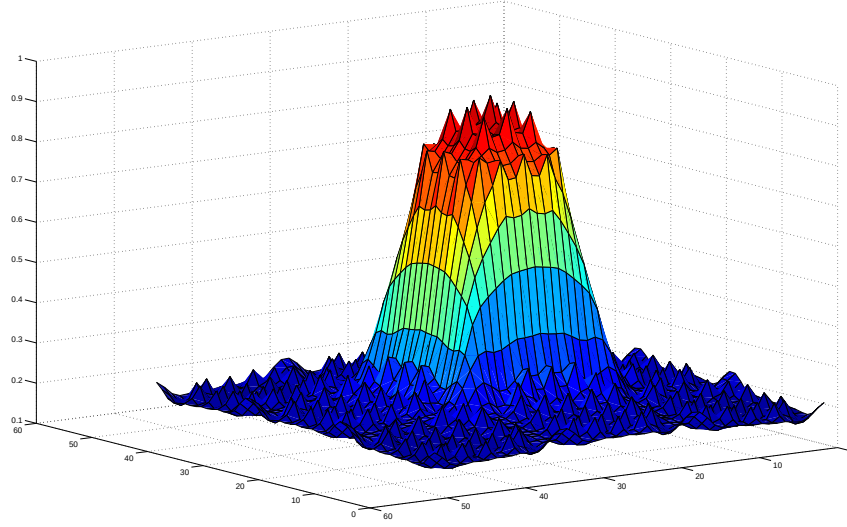
where $\mathbf{r}$ is the position vector from the origin in 2/3D, V is the volume/surface under consideration, ν is the number of neutrons released per fission, σ_{fg} is the fission cross-section in group g , ϕ_{0g} is the scalar flux in group g and G is the total number of groups. There are too many meshes per problem to effectively display the error for each case and the rms and maximum error are computed instead.

The last features of the SP_N nodal method left to be tested are the two types of diagonalisation of the SP_N formulation. In order to evaluate this both the algebraic and the similarity transform methods are tested on all cases.

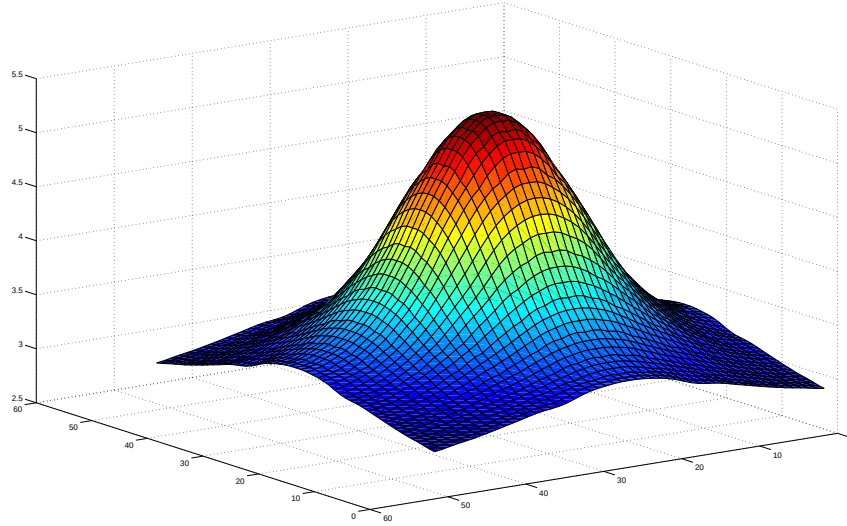
5.2.2 Results

All of the results presented in this section were produced with a fixed set of solver settings. The similarity transformation method was chosen with the original definition of the CMFD by Smith⁶. The tolerances on the flux and eigenvalue were 1.0×10^{-6} . To give some idea of the severity of the flux gradients in Case 3 the two group heterogeneous results are displayed in

fig. 5.3.



(a) Thermal



(b) Fast

Figure 5.3: The normalised fluxes for Case 3 which has the steepest gradients present.

The values of the k_{eff} for the homogeneous problems are presented in table 5.2 and table 5.3. The two group diffusion results are presented to allow comparison against PANTHER. The slight differences between PANTHER and PANTHER SP_N (PSPN) in the 2 group problems are a result of PANTHER using the ANM and PSPN the SANM. The eight group SP_7 results

Table 5.2: Coarse mesh k_{eff} values for the homogeneous EDF benchmarks with 1x1 meshes per assembly.

Groups	SP_N	Order	Code	Case 1	Case 2	Case 3
2	1	EDF		0.99997	0.99605	1.02059
		PAN		0.99995	0.99631	1.02089
		PSPN		0.99995	0.99627	1.02090
	7	EDF		0.99997	0.99710	1.02126
		PSPN		0.99996	0.99744	1.02129
8	1	EDF		0.99998	0.98978	1.01686
		PAN		0.99997	0.99000	1.01692
		PSPN		0.99997	0.99000	1.01692
	7	EDF		0.99998	0.99170	1.01795
		PSPN		0.99996	0.99201	1.01783

Table 5.3: Fine mesh k_{eff} values for the homogeneous EDF benchmarks with 4x4 meshes per assembly.

Groups	SP_N	Order	Code	Case 1	Case 2	Case 3
2	1	EDF		0.99997	0.99605	1.02059
		PAN		0.99995	0.99606	1.02057
		PSPN		0.99995	0.99606	1.02057
	7	EDF		0.99997	0.99710	1.02126
		PSPN		0.99996	0.99712	1.02121
8	1	EDF		0.99998	0.98978	1.01686
		PAN		0.99997	0.98977	1.01682
		PSPN		0.99997	0.98977	1.01682
	7	EDF		0.99998	0.99170	1.01795
		PSPN		0.99997	0.99168	1.01786

are presented to show the fidelity of the solution for higher numbers of groups and expansion orders. This subset of the k_{eff} results is representative of the whole set which deviates from the EDF results by ≈ 0.00010 for the finest mesh. This confirms that the two codes are converging to the same solution.

The values for the k_{eff} obtained from the heterogeneous cases are presented in table 5.4. Again the SP_N nodal method values for the diffusion cases, when compared against PANTHER, are almost identical. The maximum error is still ≈ 0.00010 compared to the EDF results. The errors in the flux when comparing the SP_N nodal method to the EDF results are given in

Table 5.4: k_{eff} values from performing the heterogeneous EDF benchmarks.

Groups	SP_N	Order	Code	Case 1	Case 2	Case 3
2	1	EDF		0.99999	0.99593	1.02028
		PAN		0.99992	0.99596	1.02040
		PSPN		0.99992	0.99596	1.02040
	7	EDF		0.99998	0.99700	1.02093
		PSPN		1.00000	0.99708	1.02110
8	1	EDF		0.99998	0.98971	1.01684
		PAN		0.99992	0.98974	1.01694
		PSPN		0.99992	0.98974	1.01695
	7	EDF		0.99998	0.99164	1.01788
		PSPN		0.99997	0.99166	1.01793

Table 5.5: Flux errors from performing the heterogeneous EDF benchmarks.

Case	SP_N	Order	Group	rms percentage error	max error
1	1	2		0.0209552	0.0830013
1	1	8		0.0273417	0.122101
1	7	2		0.0760936	0.347145
1	7	8		0.0575548	0.380622
2	1	2		0.096569	0.373561
2	1	8		0.0807362	0.454284
2	7	2		0.129057	0.743678
2	7	8		0.106459	0.684821
3	1	2		0.109485	0.647536
3	1	8		0.0910795	0.723256
3	7	2		0.184483	0.777888
3	7	8		0.151296	0.773016

table 5.5. The maximum pin error is less than a percent which confirms that the SP_N nodal method can obtain the correct answer to realistic colorset problems.

5.2.3 Comparison of the Different Options in the SP_N Nodal Method

The main question to address in this section is if there is any advantage to using a particular option in the SP_N nodal method. These options are the choice between an algebraic or similarity transform to diagonalise the system and the three types of CMFD. These three types of CMFD are: KS, MCNH, EDCs. The MCNH is seen as an improvement over the KS method, but

inferior to EDCs.

For the algebraic transformation the group-moment scatter matrix has negative entries meaning that the abstract fluxes can have both positive and negative values. This is a problem for both the KS and MCNH methods. There are certain values of the flux that can lead to infinite or very large values for the CMFD correction factors. This is seen in practice as most of the EDF benchmarks do not converge when using the KS method.

For this reason the MCNH method was implemented as it was less likely to introduce values into the iteration matrix which were pathological to convergence. The improvement seen was minimal as many of the EDF benchmark cases still failed. This led to the development and application of the EDCs for the SANM. A vast improvement was seen in the number of converged test cases, but the performance on realistic problems was still not reliable.

When using the similarity transformation the situation changes completely. As the group-moment scattering matrix is now entirely positive all flux solutions are positive. This gives no obvious problems for the various CMFD formulations other than those identified in the literature. The benchmark results were obtained using the KS formulation for the sake of simplicity. It is still of interest to observe if the different formulations have any impact on the solution process.

The number of power iterations, and therefore nodal updates, was recorded using the similarity transformation for both the KS and EDC formulation. The results are presented in table 5.6 and show an interesting trend. For a coarse mesh the EDC outperforms the KS formulation, while for finer meshes they are roughly equivalent. If the implementation of the EDCs can be made efficient then it is likely some performance gains will be seen on a coarse mesh.

Table 5.6: Table presenting the number of power iterations required to converge certain problems in the EDF benchmarks. These results are for Case 3 with 8 energy groups.

Order	CMFD	Meshes per Assembly			
		1x1	2x2	3x3	4x4
1	KS	71	47	45	44
	EDC	57	40	41	41
3	KS	181	115	111	109
	EDC	170	109	106	105
7	KS	230	152	144	143
	EDC	216	143	140	139

Table 5.7: k_{eff} values for the Brantley and Larsen³ test case. P_N is the spherical harmonics solution, SP_N the simplified P_N and S_N discrete ordinates with N quadrature points.

Order	EVENT	SP_N Nodal	Brantley and Larsen ³
P_1	0.77679	0.77682	0.77654
SP_3	0.79900	0.79897	0.79862
P_3	0.80012	—	—
P_5	0.80410	—	—
P_7	0.80489	—	—
S_{16}	—	—	0.80613

5.3 Brantley and Larsen Test Case

In the paper by Brantley and Larsen³ a simple test case with vacuum boundaries is proposed. This is the same case that was introduced in section 2.1 and displayed in fig. 2.1. The geometry is chosen so that the solution can be approximated well by the SP_N equations. It consists of fuel plates embedded in a moderator giving a pseudo slab geometry. The k_{eff} results are presented in table 5.7. Comparison solutions are taken from the paper and are also provided using a FEM even-parity neutron transport solver EVENT⁶⁸.

It can be seen that for this problem the SP_3 equations can predict the k_{eff} with an error of ≈ 0.001 compared to the solution of the even-parity P_3 equations. Further the SP_N nodal method agrees with both comparison values confirming the fidelity of the method.

5.4 Takeda Benchmark

The benchmarks proposed by Takeda and Ikeda⁴ are a set of 3D neutron transport problems. Model 1 is a small LWR core with homogenised cross-sections representing a void (rods-out), control rod, moderator and fuel region shown in fig. 5.4. The boundary conditions beyond the moderator are those of a bare reactor (vacuum). Model 1 is interesting because it tests many of the assumptions made when developing the SP_N nodal method. Although there are large homogenised regions with planar interfaces, which should be well captured by the SP_N equations, there are also small highly heterogeneous features. These include the void or control rod depending on the case being run. The second-order formulation also has fundamental issues when modelling a void as the transport cross-section is zero, or close to that, for a homogenised region. This issue arises because a term exists in the equations involving $1/\sigma_t$ which tends to infinity as σ_t tends to zero. In model 1 there is a small value for the cross-section in the void which mitigates this problem.

Case 1 & 2 from Model 1 were run using the SP_N nodal method with EVENT as a reference⁶⁹ and the results are displayed in table 5.8. All of the Case 2 results were obtained with the same spatial mesh, but higher-order solutions to Case 1 needed to be refined further. The convergence was also very slow for Case 1 which is not surprising as the void region is present. It can be seen that good agreement is obtained between the two codes for the SP_N results, but that there is a significant difference in the k_{eff} of ≈ 0.02 between P_N and SP_N for Case 1. Although the SP_N results are much better than diffusion in Case 1, the control rod worth would be negative for all calculations. The results show that the SP_N nodal method provides improvements over diffusion and in cases without voids this may be sufficient for application to small cores.

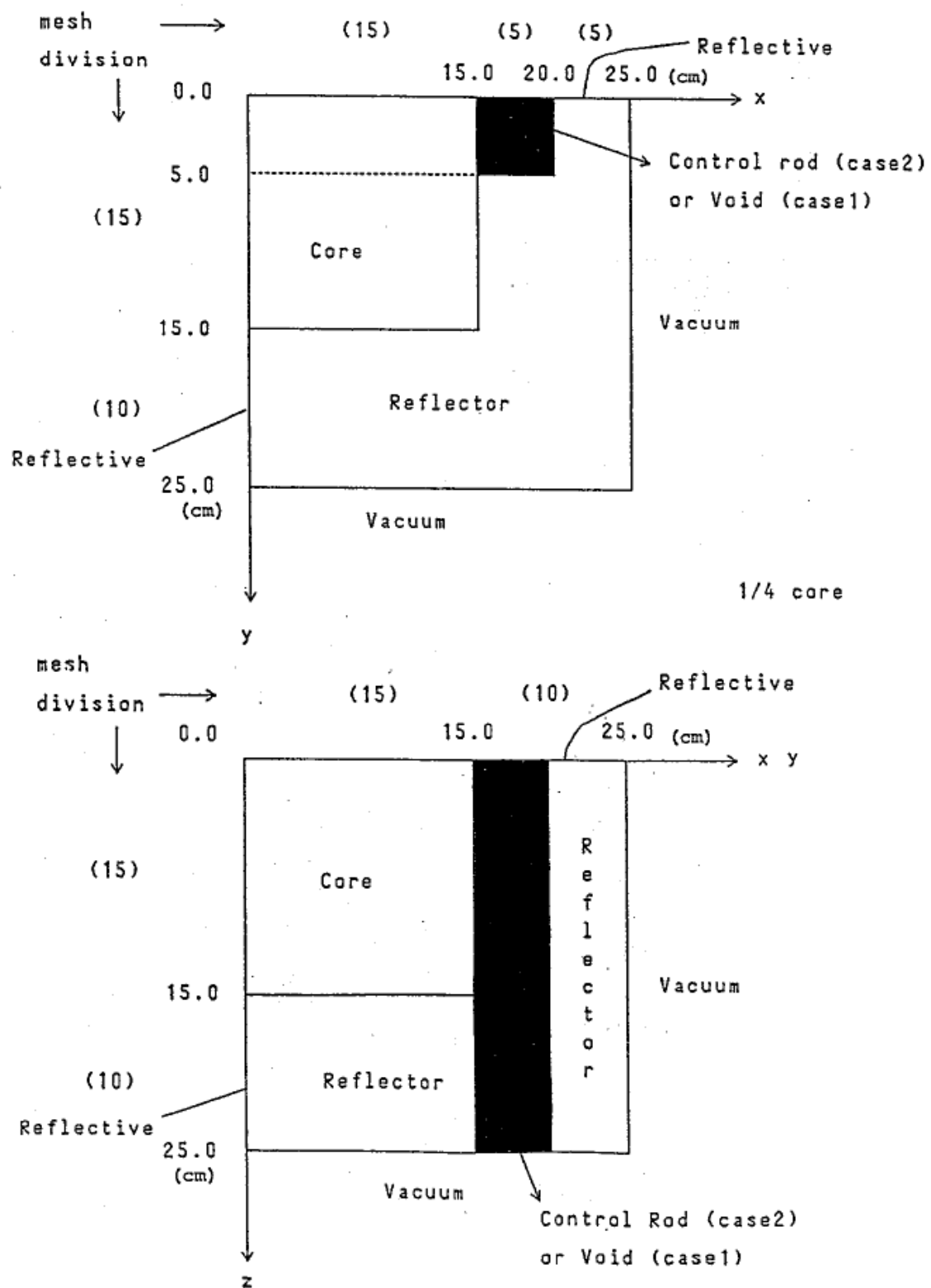


Figure 5.4: The geometry of Model 1 of the Takeda benchmark. This diagram is extracted as is from the 1991 OECD document⁴.

Table 5.8: k_{eff} values for the Takeda Benchmark. The reference solution is taken from Takeda and Ikeda⁴ and was produced using a Monte Carlo method.

Code	Order	Case 1	Case 2
Benchmark	Reference	0.9780 (± 0.0006)	0.9624 (± 0.0006)
EVENT	P_1	0.9285	0.9325
PSPN	P_1	0.9287	0.9325
EVENT	P_3	0.9725	0.9614
EVENT	SP_3	0.9558	0.9607
PSPN	SP_3	0.9558	0.9606
EVENT	P_5	0.9756	0.9623
EVENT	SP_5	0.9564	0.9615
PSPN	SP_5	0.9565	0.9614
EVENT	P_7	0.9764	0.9625
EVENT	SP_7	0.9564	0.9616
PSPN	SP_7	0.9565	0.9615

5.5 Summary

In this chapter a set of benchmarks have been performed which show that the SP_N nodal method is capable of predicting accurate solutions to a range of problems. The capability to reproduce current diffusion solutions was verified, and the extension to SP_N tested with both reflective and Mark boundary conditions.

The success of the SP_N nodal method in these benchmark cases confirms the assertions made when developing the theory in earlier chapters. It has been made clear that the similarity transformation of the SP_N equations is much more appropriate for a nodal method than the algebraic transformation. Additional stability of the EDCs is observed for the algebraic transformation and therefore their use is recommended, although further work is necessary to determine a tangible performance gain.

Now that the SP_N nodal method has been developed and tested it can be used for its intended purpose. In the following chapters it will be used as a tool to improve solutions to problems which are challenging to diffusion theory. It is hoped that the additional physical effects, modelled by the SP_N equations, will be sufficient to decreased the observed errors.

Chapter 6

The Embedded Methodology

In the previous chapters the theory of the SP_N nodal method has been developed, its implementation in the Pwr and Agr Neutronics and Thermal Hydraulics Evaluation Route (PANTHER) package described and its application to a comprehensive set of benchmarks described. In this chapter the homogenisation procedure in the embedded methodology is investigated to determine if it is valid to apply it to the SP_N equations. The embedded methodology developed by EDF Energy to correct for errors seen in the standard calculational route applied to advanced fuels, and described here, is then applied to various problems using the solution to the SP_N equations instead of the neutron diffusion equation. This was done with the aim of improving the underlying physical description through reducing the error in the solution.

The geometry and material composition of the problems addressed in this chapter are taken from the KAIST benchmark¹. This benchmark is a small Pressurised Water Reactor (PWR) core fuelled with a mixture of Uranium OXide (UOX) and Mixed OXide (MOX) fuel with an explicit baffle and reflector region. The benchmark was chosen by EDF Energy as a test of its embedded method and to this end reference solutions have been computed in Winfrith Improved Multigroup Scheme (WIMS) using the Method Of Characteristics (MOC) in 6 groups.

The overall aim of this chapter is to present step-by-step the preparation of the data required to model a full core using the modified embedded method. Once these fundamental issues have been addressed the performance of the SP_N nodal method, integrated into the embedded methodology, can be evaluated.

In section 6.1 the homogenisation procedure is discussed and a pincell correction factor is derived for the SP_N equations. The homogenisation procedure is then tested on a line of pincells which is representative of interfaces between MOX and UOX assemblies in a reactor core. Section 6.2 describes how the pintype correction factors for a full assembly are computed using Single Assembly (SA) Infinite Lattice Calculations (ILCs) for use in the 6 group pin-by-pin calculations of the embedded methodology. The pintype correction factors computed in the SA calculations are then utilised in colorset calculations in section 6.3. These colorset calculations are analysed to determine the impact of using the SP_N nodal method instead of a diffusion model in the embedded method. The final step in the analysis is to model the full quarter core of the KAIST benchmark in section 6.4. This is to determine the benefits of including an approximate transport model in a realistic problem.

6.1 Homogenisation

It has been proposed that the SP_N equations are solved, as a replacement for the diffusion equation, in the embedded method. It is therefore necessary to investigate if the existing homogenisation procedure is adequate for use with the SP_N equations. The homogenisation procedure is used to preserve the reaction rates and leakages from a SA ILC in a full core calculation with homogeneous assemblies, and reassemble the pin powers. Generalised equivalence theory²⁵ has traditionally been seen as the most accurate means to homogenise data for use

in reactor core calculations. This is a very practical method to homogenise assemblies using SA ILCs as it results in one correction factor per group for each assembly. This correction factor is a discontinuity factor for the scalar flux that is chosen to preserve the flux value on the boundary from the reference calculation.

The process of homogenisation has been revisited recently by Sanchez⁹. It is highlighted that it could be better to introduce correction factors that preserve the partial currents on the boundary of a region, in place of flux discontinuity factors that preserve the boundary fluxes. For the case of SA homogenisation using ILCs it is found that this can be achieved using a single factor per group as in Generalised Equivalence Theory (GET). The definition of these factors is significantly different from the definition in GET which was made to preserve averaged quantities from a reference model, which was also diffusion. In the specific case of a diffusion operator for both the reference and homogeneous models the two correction factors are equivalent. However, when the higher-order model is transport theory then the definitions differ. It was found that the definition which preserves the partial currents gives more accurate results than those of GET.

When analysing MOX-UOX fuelled cores the homogenised data is derived in a reference situation that can be very different from that experienced in the reactor. There can be large leakages and changes in the spectrum due to neighbouring assemblies, which are not present in the ILC. It is therefore necessary to understand the impact of homogenisation in a problem where the assumptions made during homogenisation are stretched. In order to do this a simple geometry is chosen, that of a line of pincells. The solution of this problem will give some indication of the best possible performance of a homogenisation technique. The subsequent developments can then be viewed as the application to realistic problems.

The line of pincells consists of 10 identical MOX pincells adjacent to 10 identical UOX pincells.

The pincell enrichments are chosen to make the interface difficult to compute to highlight the physics processes going on. The analogue to an ILC in this situation is chosen to be a calculation of one fuel pin and its surrounding moderator in an infinite lattice. This allows extraction of homogenised cross-sections which preserve the reaction rates, and surface fluxes or currents for computing the correction factors. Effectively each pin type will be collapsed and smeared in its own spectrum, which is different from that of the full line of pincells.

In order to preserve the reaction rates when using the SP_N equations the same homogenised cross-sections can be used as for the diffusion equation. This is not true, however, when considering anisotropy of collision. In this case homogenised parameters need to be defined for the higher moments of the angular flux. A method to do this has been presented by Sanchez⁹, but it requires values for the higher moments of the angular flux which are not available in WIMS. The SP_N nodal method does not include anisotropic scatter and these cross-sections would not be used even if they could be defined.

The ease of application of correction factors which preserve the partial currents, coupled with the results presented in the literature⁹, has led to this method being adopted in the line of pincells. Sanchez⁹ goes further and defines correction factors for the SP_N equations that will preserve the angular moments of the P_N boundary fluxes. This would in theory allow the angular dependence of the neutron flux to be preserved in some capacity, not just the average value of the current. However, this also requires the higher moments of the angular flux from the reference transport calculation which are not available.

In order to apply corrections to the SP_N equations one can instead ask that the physical current, the first angular moment, is preserved. This leads to a definition of one correction factor per energy group that is applied to *all* even angular moments. It turns out that this can be implemented in exactly the same way as in diffusion theory. This means that the framework,

which exists in PANTHER, can be used to apply this correction factor.

6.1.1 Pincell Correction Factor for the SP_N Equations

In slab geometry the partial current for the SP_N equations is given by

$$\int_{\mu \gtrless 0} \mu \left[\overline{\psi}^+(x, \mu) - \frac{\mu}{\bar{\sigma}} \frac{\partial}{\partial x} \overline{\psi}^+(x, \mu) \right] d\mu \bigg|_{x \in \Gamma} = \overline{J}_{\pm}, \quad (6.1)$$

where the quantities with a line such as $\overline{\psi}$ refer to the homogenised problem, $J_{\pm}$ is the partial current in the right and left direction, and Γ is the boundary. This equation is the definition of the partial current in the even-parity formulation of the neutron transport equation in slab geometry. This can be expanded in terms of the even normalised Legendre polynomials as in section 2.3:

$$\int_{\mu \gtrless 0} \mu \left[\sum_{\substack{l=0 \\ l \in \text{even}}}^{\infty} \overline{\psi}_l(x) p_l(\mu) - \frac{\mu}{\bar{\sigma}} \frac{\partial}{\partial x} \sum_{\substack{l=0 \\ l \in \text{even}}}^{\infty} \overline{\psi}_l(x) p_l(\mu) \right] d\mu \bigg|_{x \in \Gamma} = \overline{J}_{\pm}. \quad (6.2)$$

The ILC has the property that $|\overline{J}_+| = |\overline{J}_-|$ and therefore the above expression can be reduced to

$$|\overline{J}_{\pm}| = \int_0^1 \mu \sum_{\substack{l=0 \\ l \in \text{even}}}^{\infty} \overline{\psi}_l(x) p_l(\mu) d\mu \bigg|_{x \in \Gamma}. \quad (6.3)$$

The above expression relates the partial currents $|\overline{J}_{\pm}|$ and the moments of the angular flux $\overline{\psi}_l$ from the homogeneous problem evaluated at the boundary. The issue identified with homogenisation is that when the reaction rates are preserved the partial currents do not match those of the higher-order transport solution. This results in the leakage being computed incorrectly and the eigenvalue not being preserved.

This can be corrected for in a simple fashion for the SP_N equations in slab geometry. A correction factor f can be multiplied by *all* of the even moments of the flux to ensure that the

leakage from the cell is correct. This results in

$$J_{\pm} = f \overline{J_{\pm}} = \int_0^1 \mu \sum_{\substack{l=0 \\ l \in \text{even}}}^{\infty} f \overline{\psi_l}(x) p_l(\mu) d\mu \bigg|_{x \in \Gamma}, \quad (6.4)$$

where $J_{\pm}$ is the heterogeneous transport partial current. In fact, for a homogeneous problem, all higher moments of the angular flux are zero and the expression simplifies further to that given by Sanchez⁹ for the diffusion equation

$$J_{\pm} = \frac{f \overline{\phi}}{4}, \quad (6.5)$$

where $\overline{\phi}$ is the boundary value of the scalar flux in the homogeneous problem. This expression defines f given the heterogeneous transport current and the scalar flux solution of the homogeneous problem. Once eq. (6.5) has been used to define the correction factor f , it is applied according to eq. (6.4). The assumption is that it is valid to apply the same correction to all higher-order even angular moments. This makes the implementation easier as f is the same as in the diffusion case and can be implemented by the existing PANTHER framework.

The important result of this analysis is that a single correction factor per group is required to preserve the partial currents in the homogeneous case for the SP_N equations. This is identical to the existing treatment in PANTHER, albeit with a different definition of f . The framework for the application of discontinuity factors from GET can be used to implement partial current conservation.

6.1.2 Results for a Line of Pincells

The test problem chosen by EDF Energy is the MOX-UOX line where the MOX is enriched to 8.7% and the UOX to 3.3% as in the KAIST benchmark¹. In order to prepare nuclear data and reference solutions for this problem WIMS has been used. Four calculations are performed:

1. Collision Probabilities (CP) in 172 energy groups for each heterogeneous single pincell to collapse the data to 6 energy groups. This is followed by the MOC in 6 energy groups to provide a flux to spatially homogenise the cross-sections in a pincell. The solution is also used to compute correction factors for the homogeneous problems.
2. MOC with heterogeneous pincell geometry for the full line in 6 groups using unsmeared condensed data from the single pincell calculations. This results in a practical reference solution to investigate how well particular cross-section definitions perform. This is the case that the correction factors are computed to reproduce.
3. MOC with homogenised pincell geometry in 6 groups for the full line using the smeared data from the single pincell calculations. This results in a reference solution to the approximate geometry to verify that any transport solver is functioning correctly.
4. MOC in 172 groups for the heterogeneous line problem. This is the reference solution to which we are trying to compute an approximation. The difference between this solution and the heterogeneous MOC in 6 groups represents an error that cannot be removed using the homogenisation procedure. It is not practical to perform ILCs in the full 172 groups for production runs due to the number of such calculations required.

Various calculations are performed with PANTHER and the SP_N nodal method to better understand the impact of the various approximations made in the data preparation and codes used. The quantities of interest are the eigenvalue, 6 group fluxes and pin powers for the line of pincells. The smeared and collapsed data from WIMS calculation 1 is used for all cases. The four homogeneous calculations are:

1. PANTHER without correction factors,
2. PANTHER with correction factors to preserve the partial currents,
3. SP_N nodal method without correction factors,
4. SP_N nodal method with the same correction factors used for the diffusion case.

The spectrum that the cross-sections have been collapsed in will not be correct in the vicinity of the interface, which will add errors which cannot be removed by homogenisation. This will be somewhat alleviated by the increased number of groups. The main point of this test is

Table 6.1: Results of running homogeneous calculation 3 and comparing against WIMS calculation 3. The fidelity of these results indicates that the nuclear data is being transferred to PSPN correctly and that the transport solution is correct.

Quantity	WIMS	PSPN
k_{eff}	1.225759	1.225754
max. flux error	-	0.091%
max. power error	-	0.041%

threefold. Firstly, to determine that the data is being imported correctly from the lattice cell code. Secondly, to quantify the sizes of the errors between a diffusion and transport calculation, and how well the SP_N nodal method can capture this type of problem. The expectation is that in slab geometry SP_N should converge to the same solution as WIMS calculation 3 due to the equivalence of the P_N and SP_N equations in slab geometry. Thirdly, to observe the impact of using the correction factors.

The results of running homogeneous calculation 3 for SP_{21} are given in table 6.1. These results confirm that the SP_{21} calculation is capable of obtaining the transport solution in slab geometry and converges to the same answer as the MOC. It also confirms that the nuclear data has been accurately imported into PANTHER SP_N (PSPN).

In figs. 6.1 to 6.6 the 6 group flux solutions are displayed which are a result of using the data from WIMS calculation 1 in the various codes. The comparison here is done against WIMS calculation 2 which is expected to be a good approximation to the true reference solution, and which the homogeneous calculations are designed to reproduce. At the highest energies the errors are similar for diffusion and SP_3 , but at thermal energies significant differences can be seen between the two models. It should be noted that size of the errors in the pin powers for PSPN with and without the correction factors were similar, and the uncorrected results are displayed here. There was an impact on the error due to the correction factor in the SP_3 thermal fluxes, but this did not carry through to the pin powers.

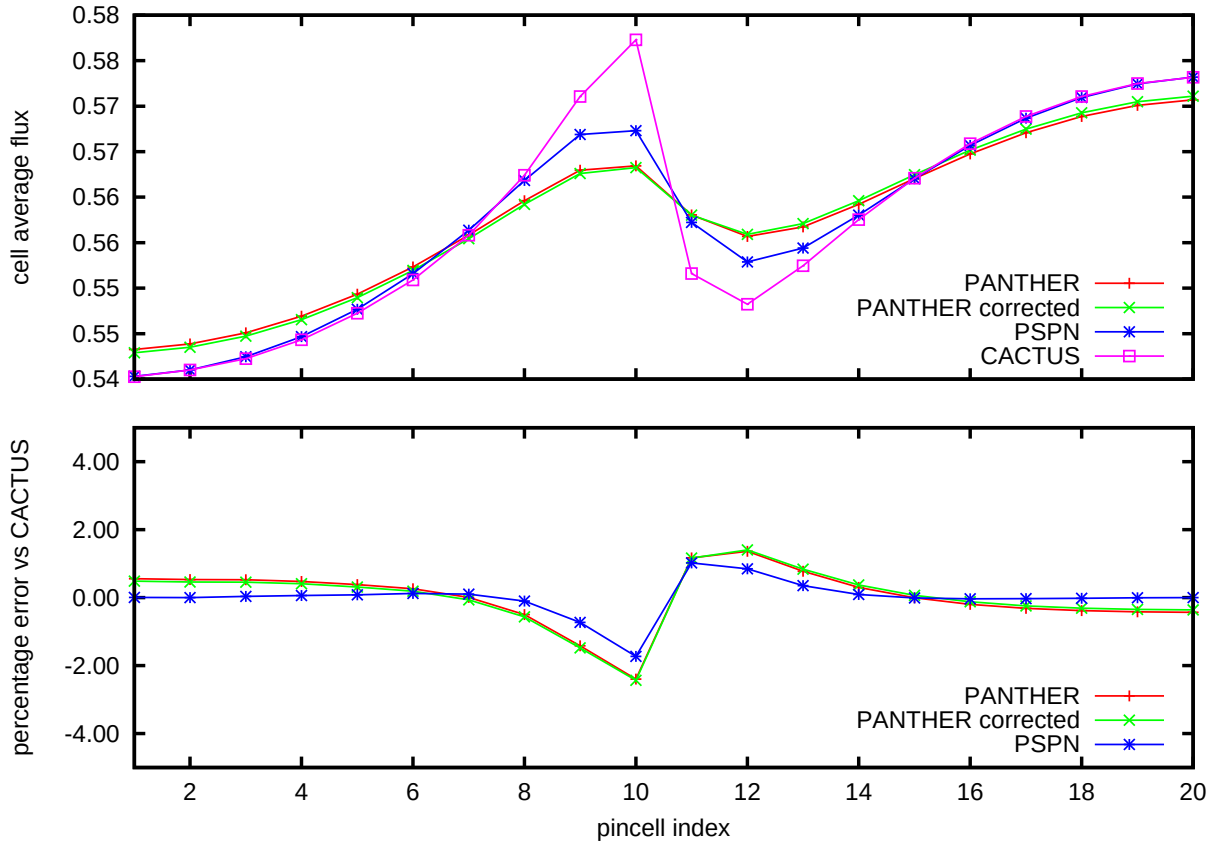


Figure 6.1: The flux profile for the highest energy group 1 of the homogeneous line problem is shown in the upper plot. The corresponding errors are shown in the lower plot. The differences between a transport (CACTUS), P_3 (PSPN) and diffusion (PANTHER) solution are highlighted. The largest errors occur at the interface, pins 10 and 11, for the diffusion case. Relatively large errors are also seen in the P_3 results.

In order to see the impact on a quantity of interest, the errors in the pin power values are displayed in fig. 6.7. The sensitivity of the pin powers to the thermal fluxes can clearly be seen here. For the uncorrected diffusion model the errors in the highest and thermal groups are of the same order and this leads to a significant error in the pin power. For the P_3 model, the highest errors are in the fast group and the impact on the pin powers is minimal.

It is interesting to note how close the corrected PANTHER results are to those of PSPN. It appears that the two models correct for essentially the same effects, but are incapable of removing the last few percent of error. This is understood to arise from collapsing the nuclear data in the wrong spectrum, and the loss of geometric information in the homogeneous problem.

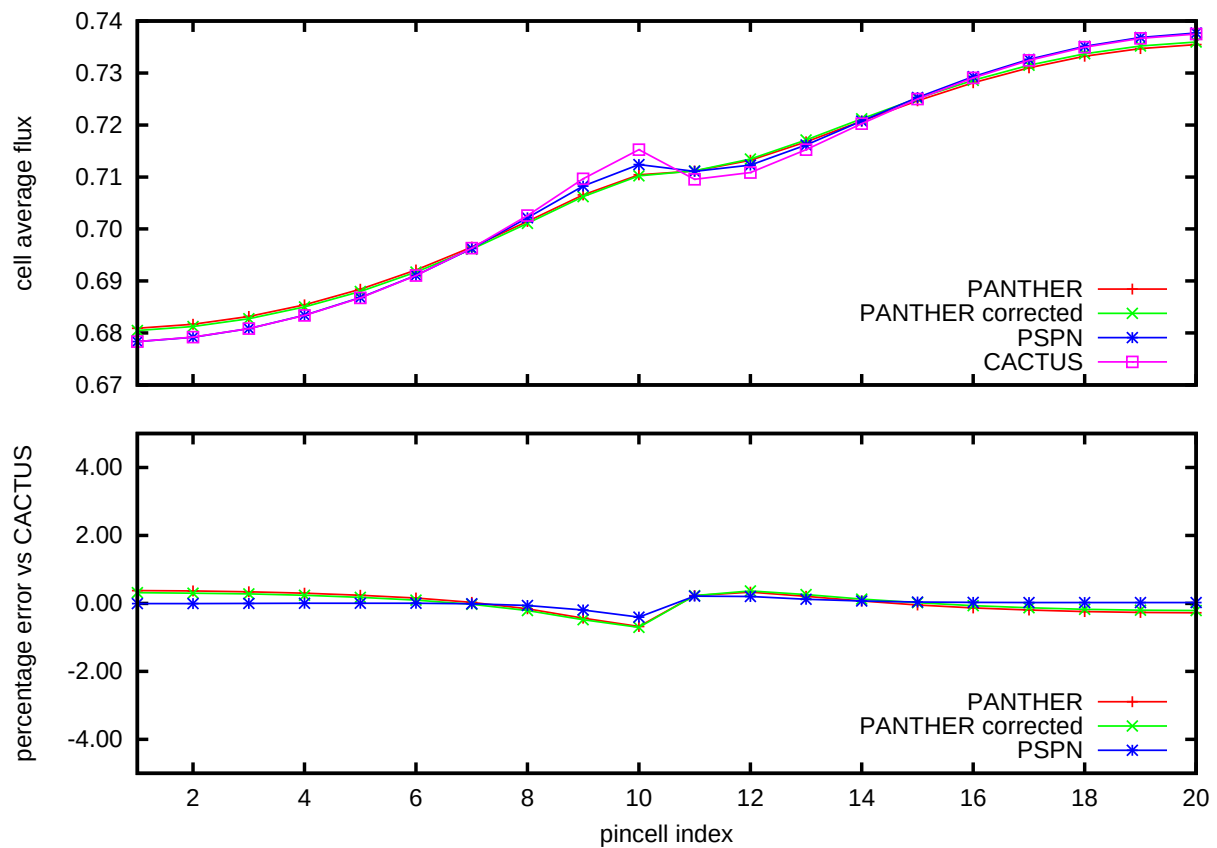


Figure 6.2: The flux profile for energy group 2 of the homogeneous line problem is shown in the upper plot. The corresponding errors are shown in the lower plot. In this energy group the errors are of modest size.

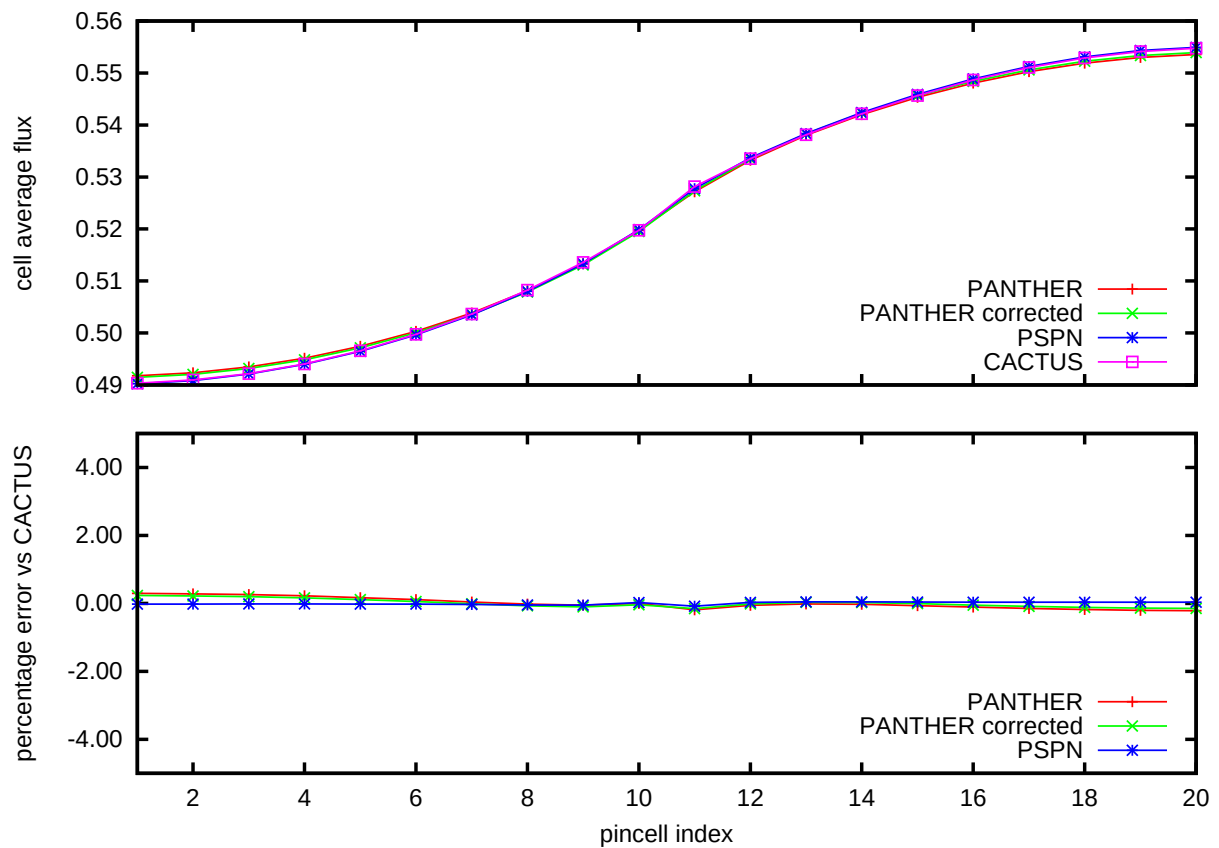


Figure 6.3: The flux profile for energy group 3 of the homogeneous line problem is shown in the upper plot. The corresponding errors are shown in the lower plot. In this energy group the errors are of modest size.

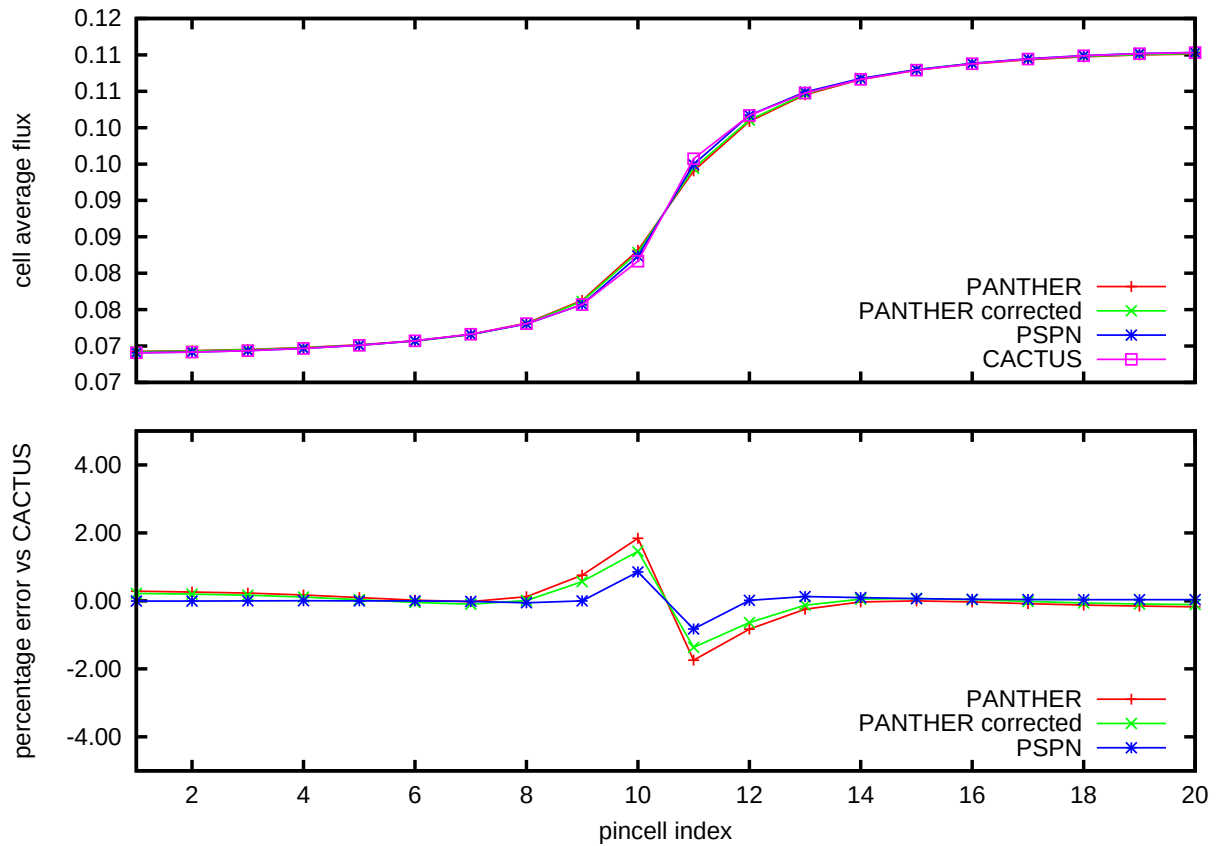


Figure 6.4: The flux profile for energy group 4 of the homogeneous line problem is shown in the upper plot. The corresponding errors are shown in the lower plot. The differences between a transport (CACTUS), P_3 (PSPN) and diffusion (PANTHER) solution are highlighted. As the thermal energy region is approached, errors begin to re-appear at the interface, pins 10 and 11, and are larger for the diffusion model.

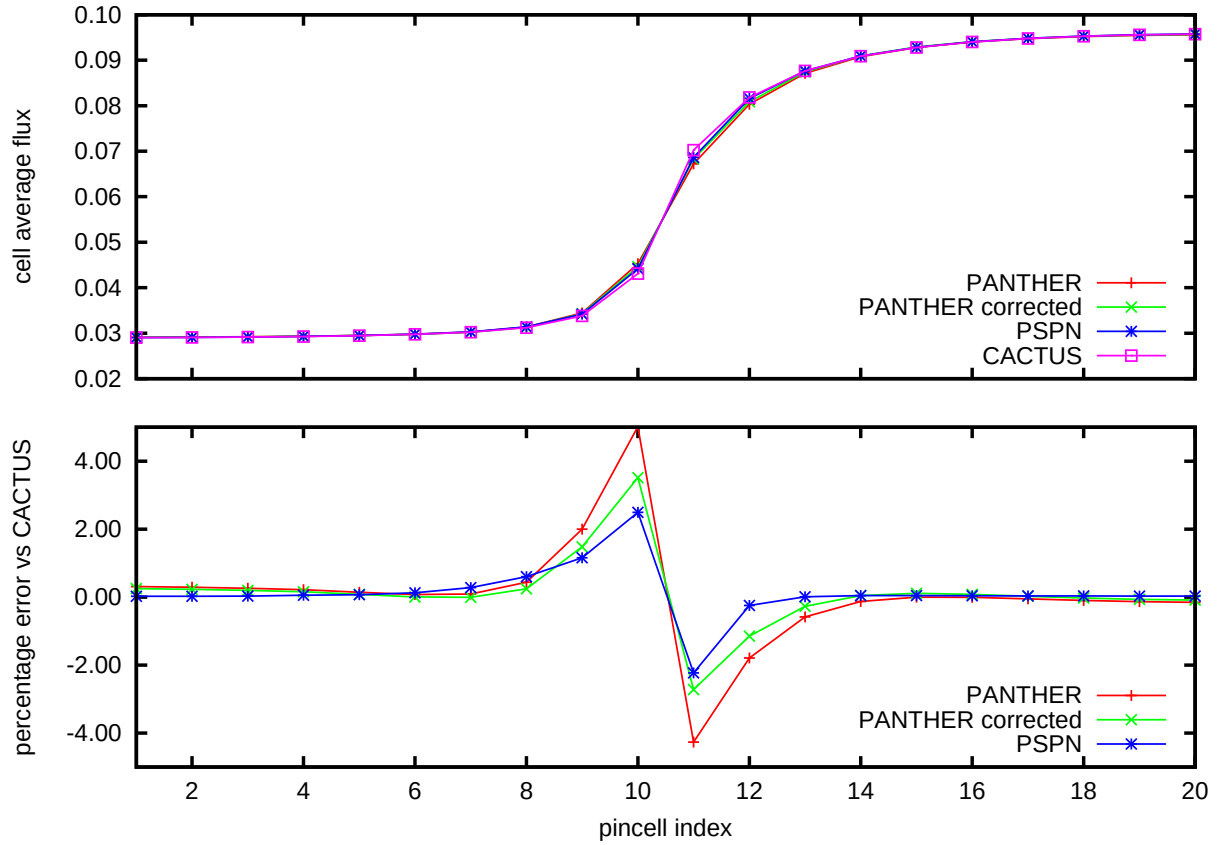


Figure 6.5: The flux profile for energy group 5 of the homogeneous line problem is shown in the upper plot. The corresponding errors are shown in the lower plot. The differences between a transport (CACTUS), P_3 (PSPN) and diffusion (PANTHER) solution are highlighted. Large errors occur at the interface, pins 10 and 11, for the uncorrected diffusion case.

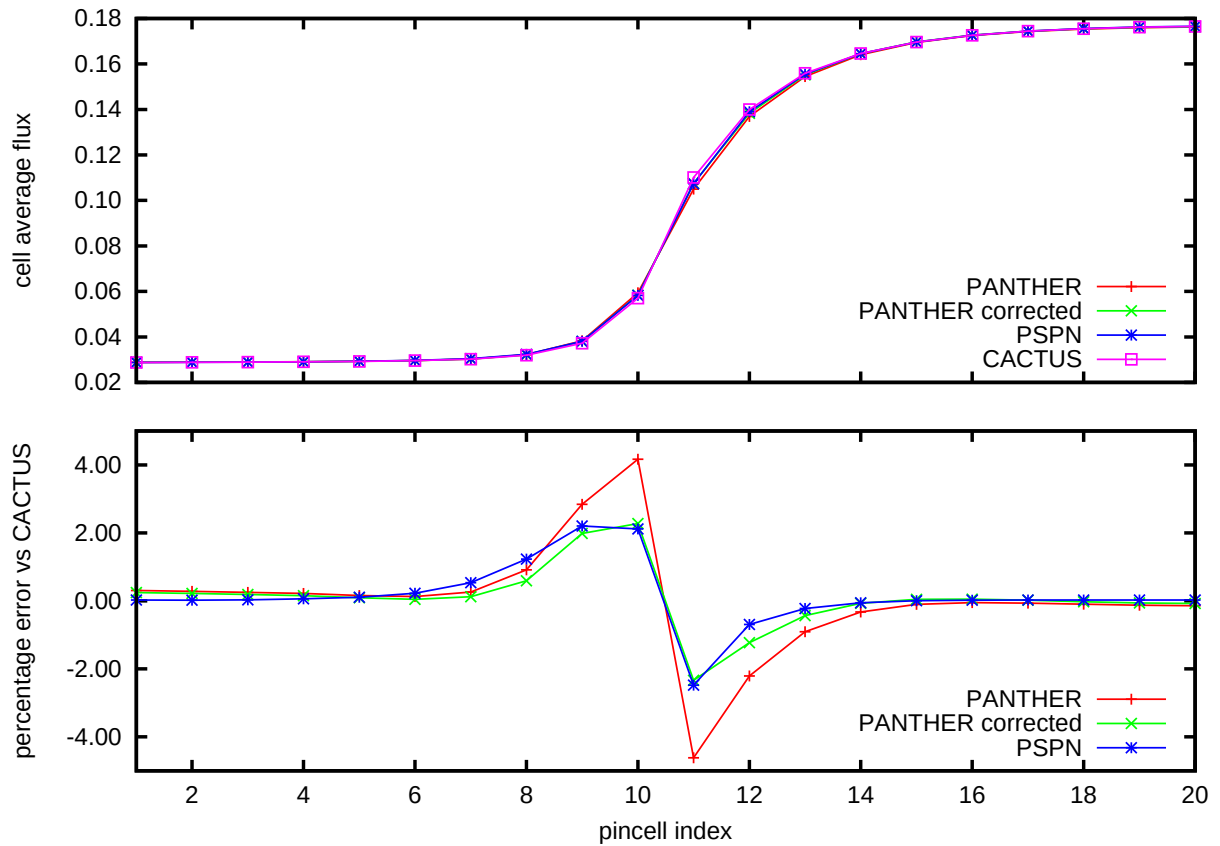


Figure 6.6: The flux profile for the lowest energy group 6 of the homogeneous line problem is shown in the upper plot. The corresponding errors are shown in the lower plot. The differences between a transport (CACTUS), P_3 (PSPN) and diffusion (PANTHER) solution are highlighted. The trend of large errors in the uncorrected diffusion solution for thermal energies at the interface, pins 10 and 11, holds.

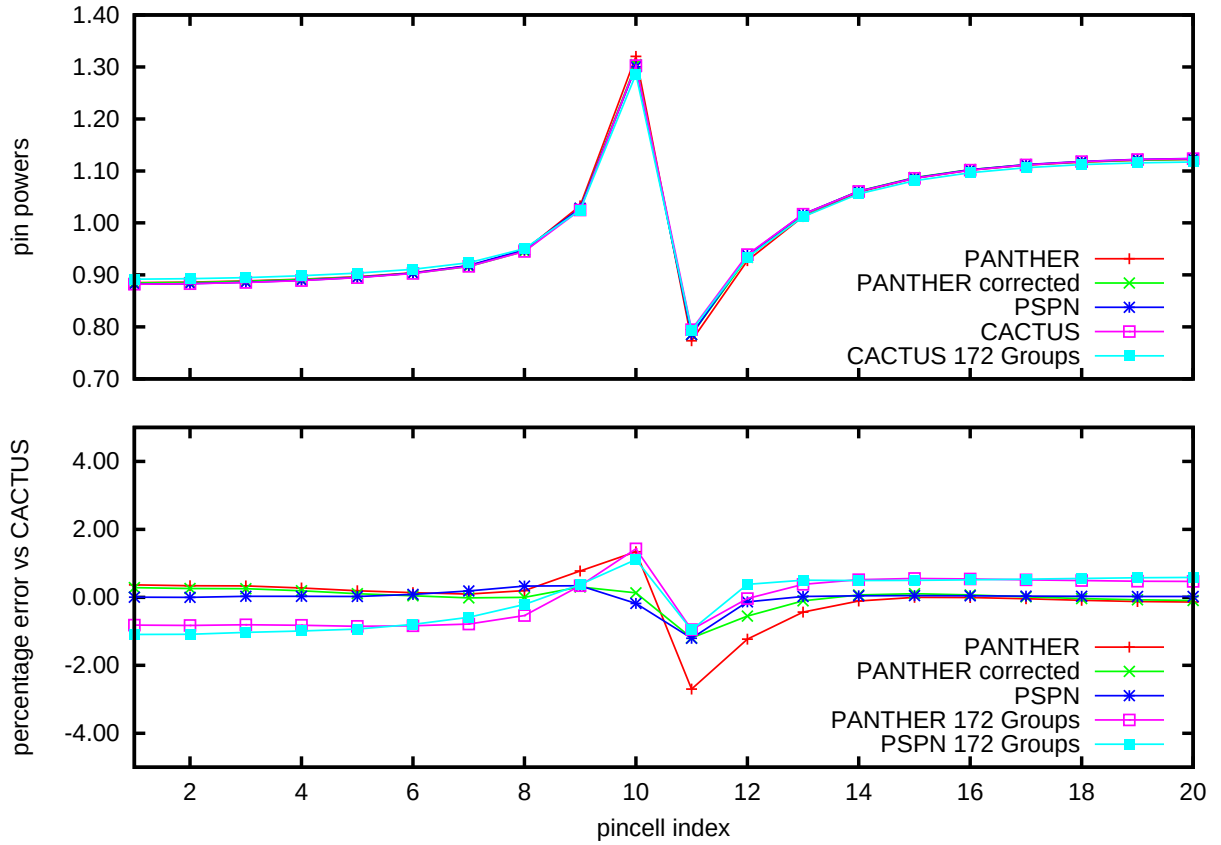


Figure 6.7: The pin powers are shown to display the decrease in the errors when using the corrected diffusion (PANTHER) and P_3 (PSPN) methods, compared to WIMS calculation 2 (explicit geometry in 6 groups). The sensitivity of the pin power errors to the error in the thermal fluxes can also be observed when comparing to the individual group fluxes. Although the error in the fast flux remains at $\approx 2\%$ the thermal flux errors are much lower for the corrected diffusion and P_3 methods, and correspondingly the error in the pin powers is very low. The 172 group results are comparisons against WIMS calculation 4.

The last step in the analysis is to determine the differences in the solutions to the homogeneous problems and the 172 group reference solution in WIMS calculation 4. In fig. 6.7 these comparisons are presented. It can be seen that these errors are of the order of the error on the interface, and we are therefore doing the best that can be reasonably expected due to practical constraints. The impact of using the correction factors can also be seen. It is evident that it is worth applying correction factors for diffusion even in cases that deviate significantly from the assumptions made in the ILC.

There is a second class of problem where some interesting results can be observed. The same calculational route is used as before, but the two pincell types are 2.0% and 3.3% enriched UOX. This is significantly different as the spectrum in which each pincell is collapsed is similar and should be very close to that of the full line problem. The second feature is that the correction factors, which should preserve partial currents, are close to unity compared to those computed for the MOX-UOX line and therefore have little effect.

The group fluxes for the problem with an enrichment change are given in figs. 6.8 to 6.13. It can be seen that in the bulk of the material (away from the interface in pincells 1 and 20) there is very good agreement between PSPN and WIMS. The diffusion model with and without correction factors, however, cannot correctly capture the reaction rates. It is expected that in the bulk the reaction rates should be accurate, with the use of correction factors. What the diffusion model is failing to capture is a large leakage of neutrons from one material to the other. In order to obtain an accurate homogenisation the currents resulting from this leakage would need to be applied as boundary conditions to the ILCs, this of course is not practical as it requires the full solution in advance. On the interface there are still errors from homogenisation of $<0.5\%$, but these are dwarfed by the error in the bulk.

The pin powers are shown in fig. 6.14 and the same trends can be seen as in the group fluxes. The

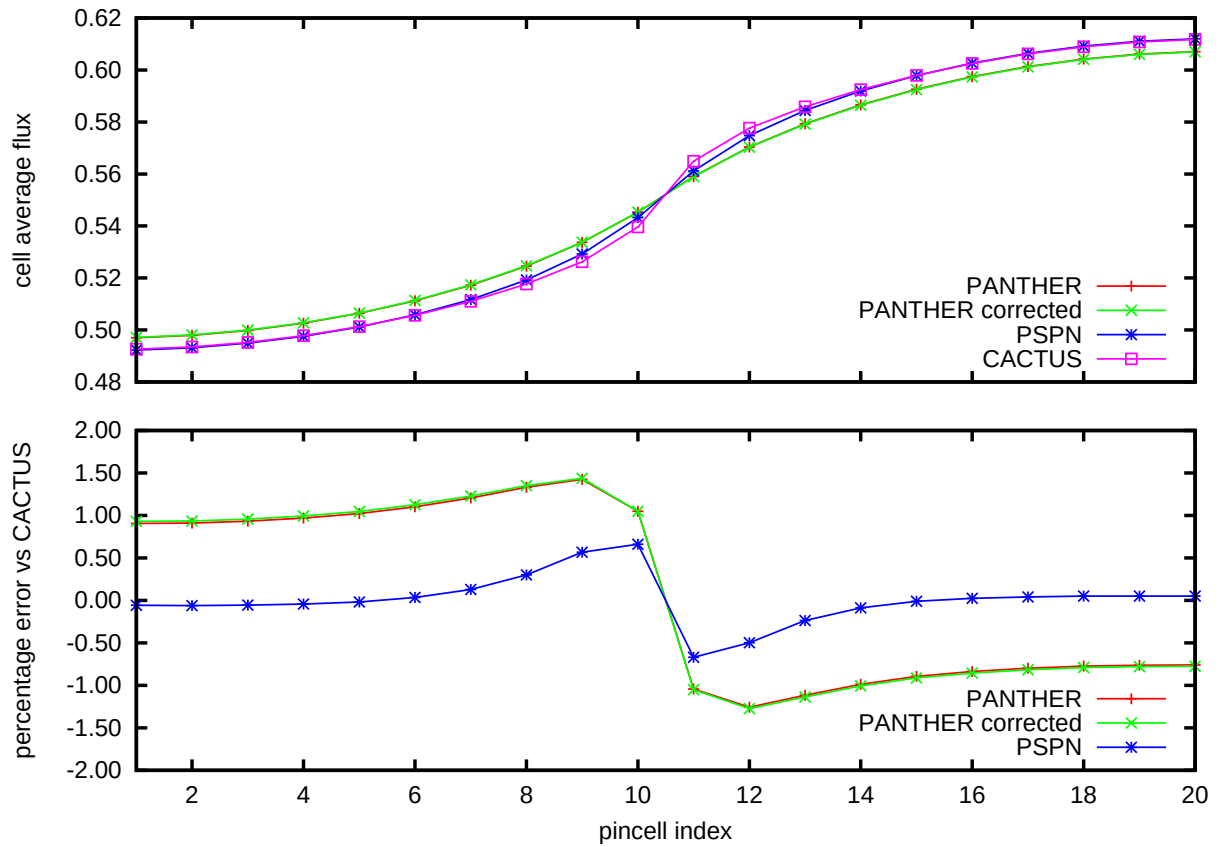


Figure 6.8: The flux profile for the highest energy group 1 of the enrichment change problem. It can be seen that in the bulk of the material (pincells 1 and 20) there is very good agreement between PSPN and WIMS.

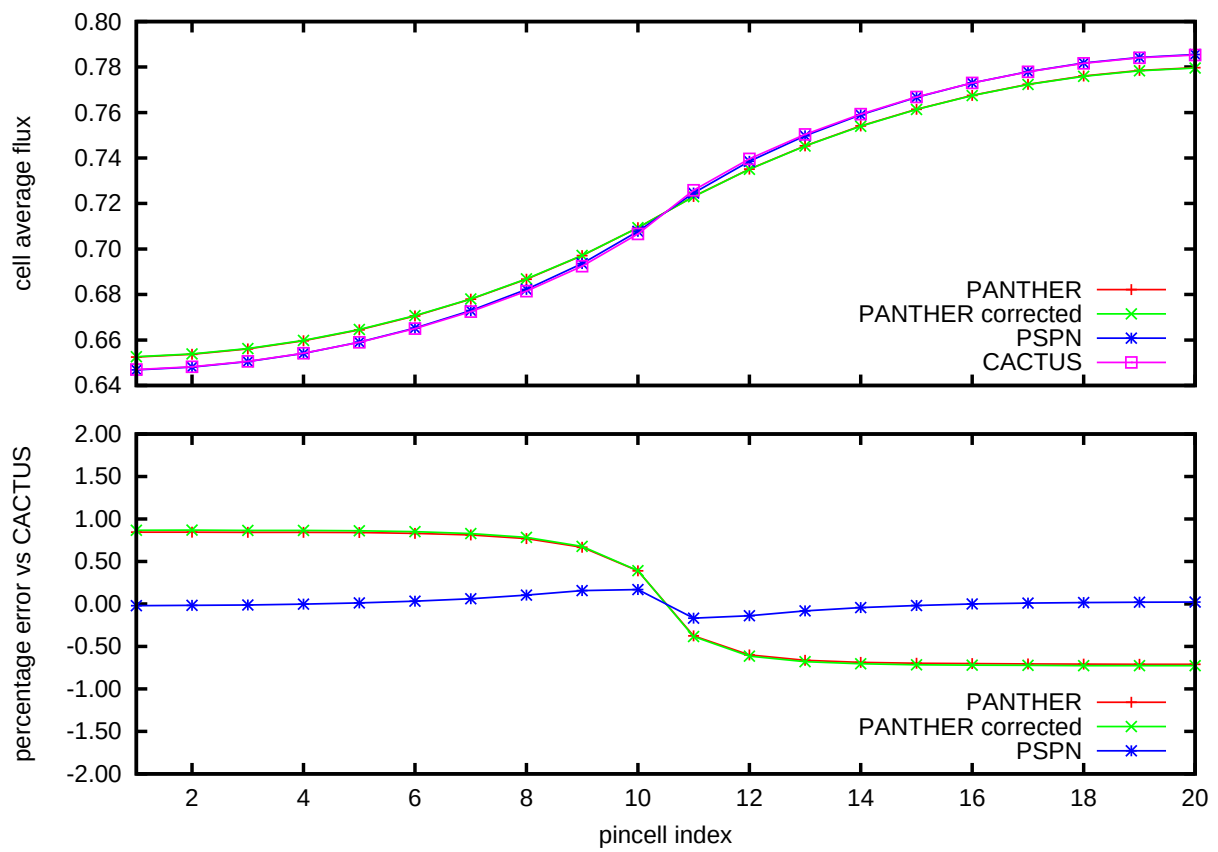


Figure 6.9: The flux profile for energy group 2 of the enrichment change problem.

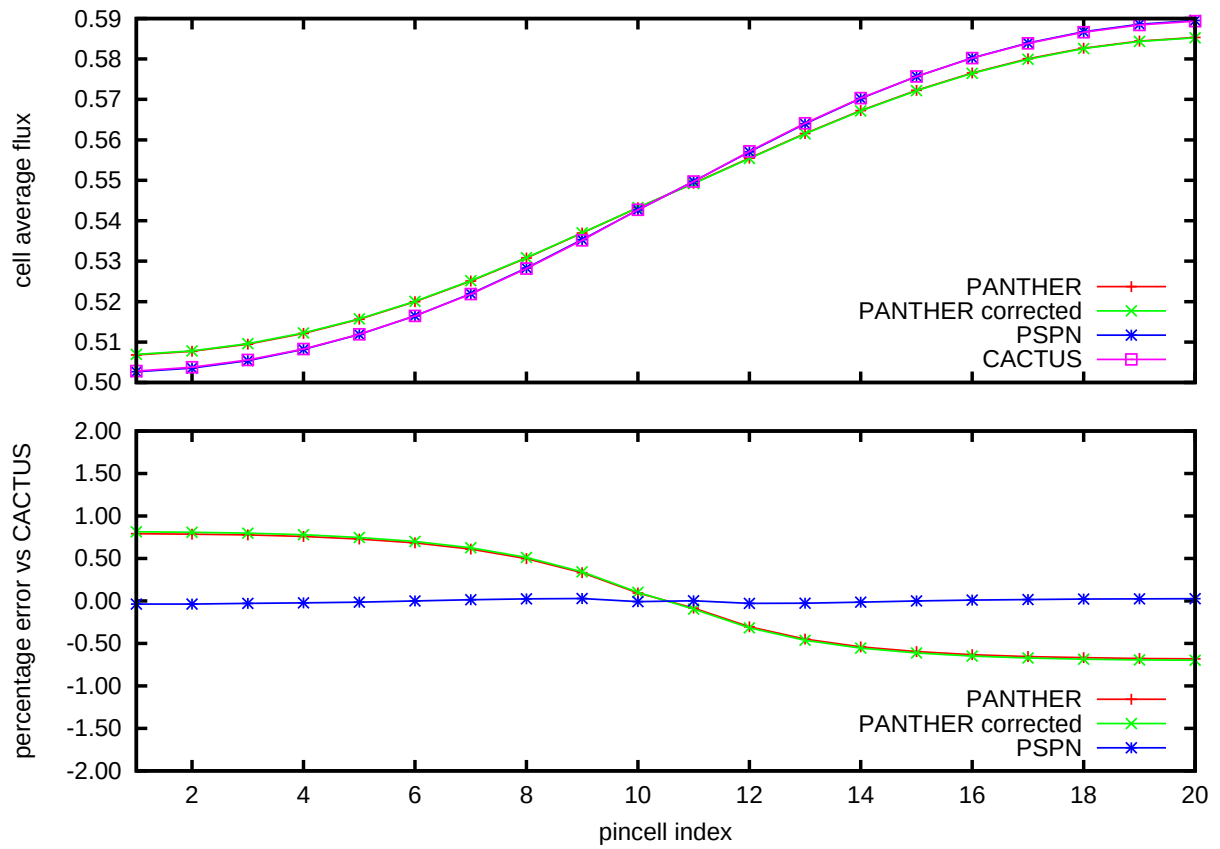


Figure 6.10: The flux profile for energy group 3 of the enrichment change problem.

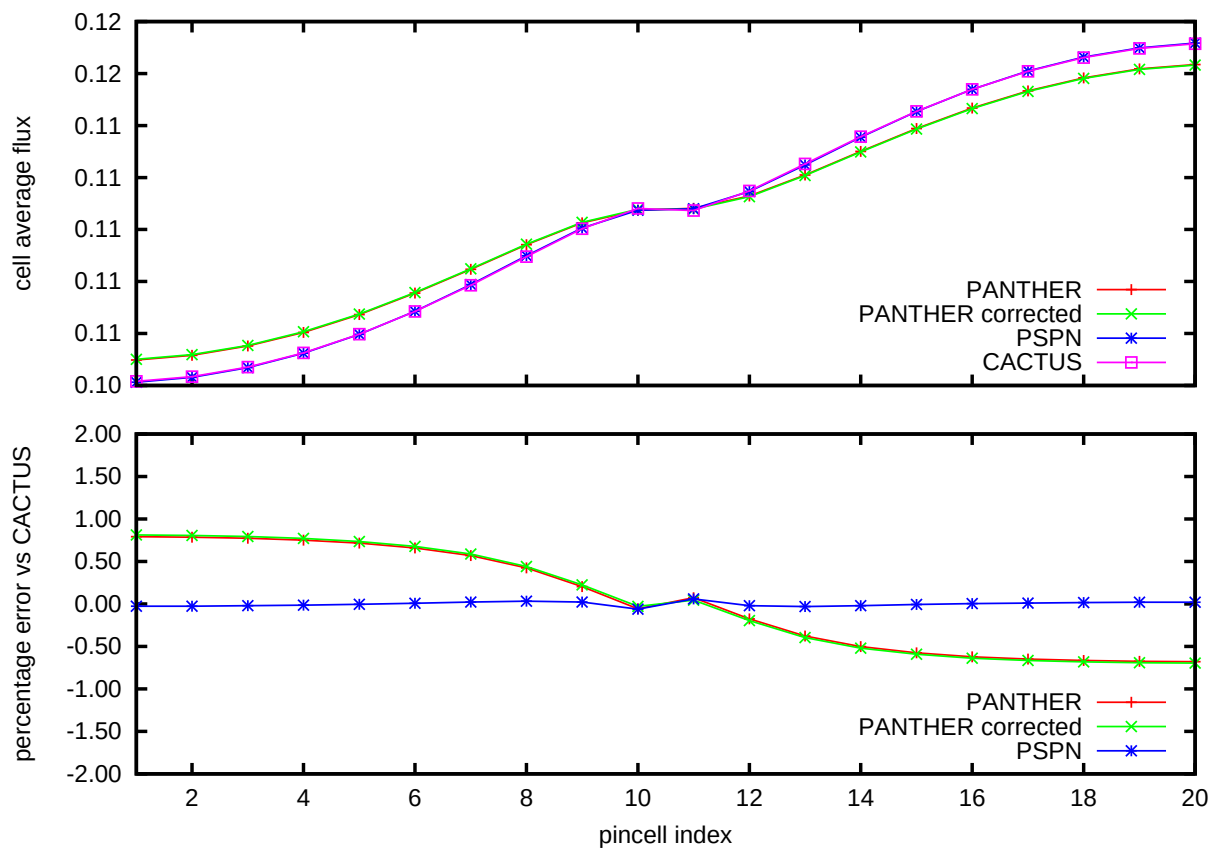


Figure 6.11: The flux profile for energy group 4 of the enrichment change problem.

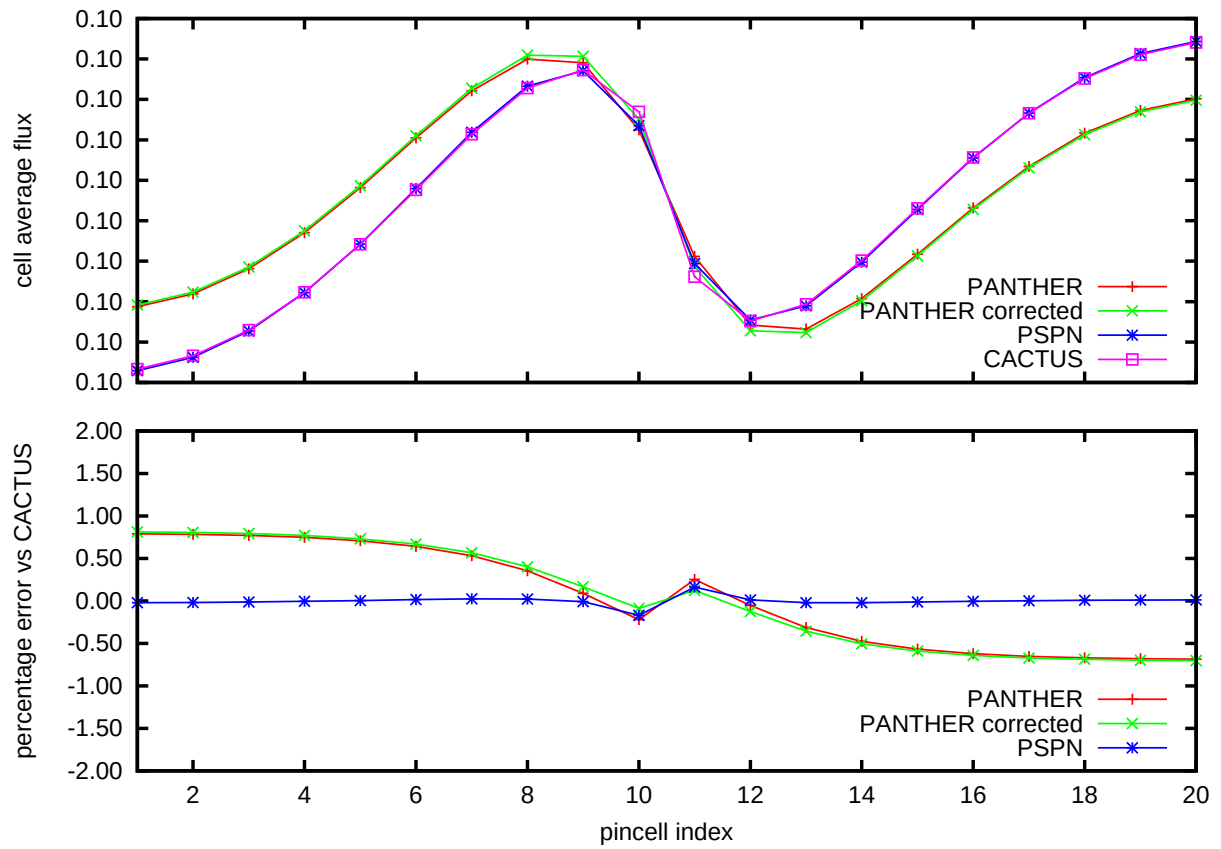


Figure 6.12: The flux profile for energy group 5 of the enrichment change problem.

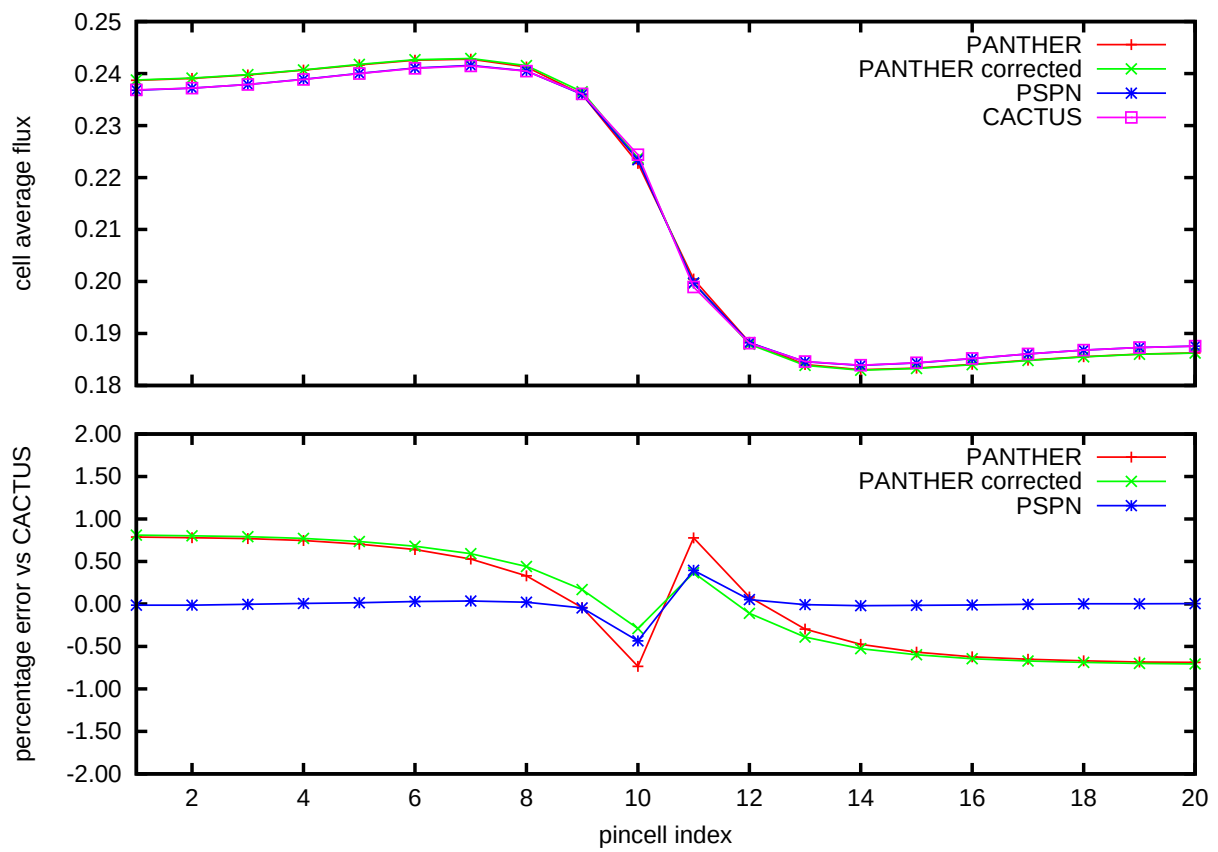


Figure 6.13: The flux profile for the lowest energy group 6 of the enrichment change problem.

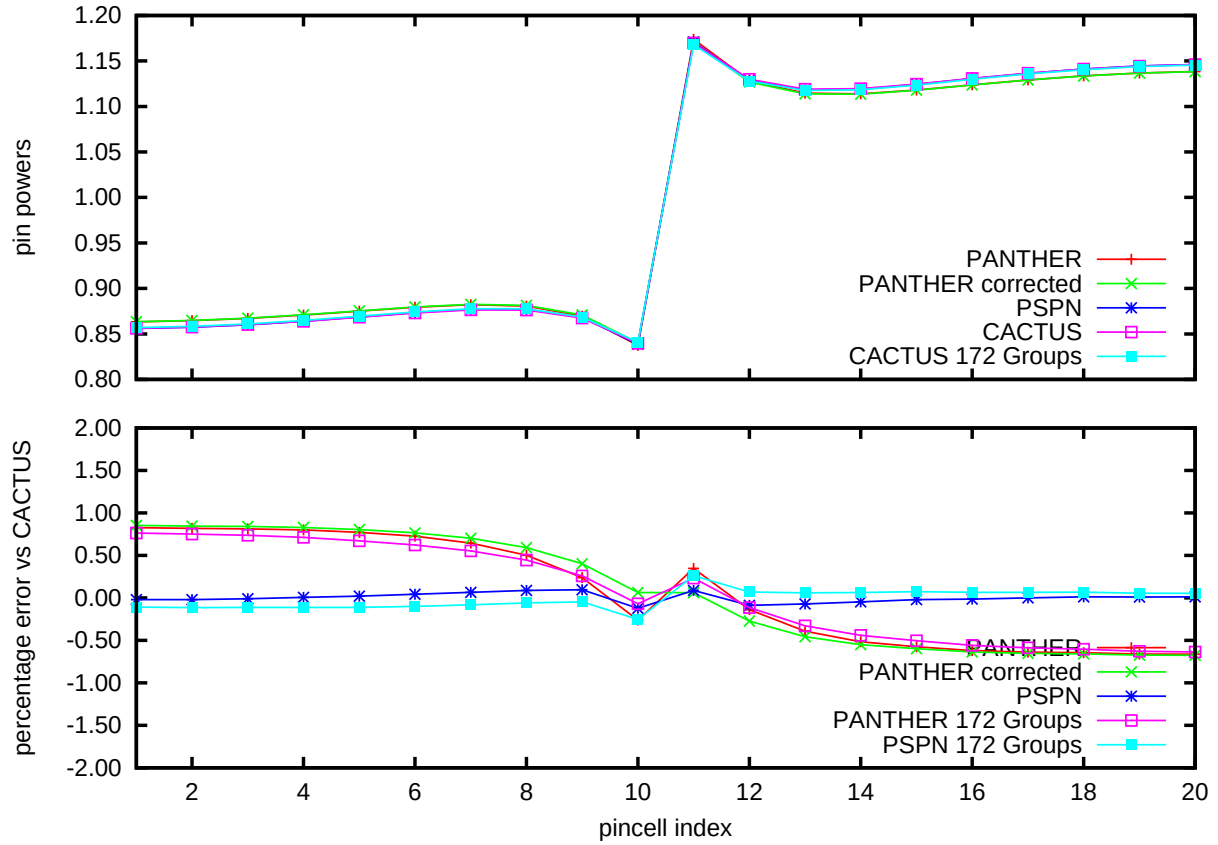


Figure 6.14: The CACTUS results are computed in WIMS calculation 2 (explicit geometry in 6 groups) and used to compute the errors in the solutions. The 172 group results are all derived from WIMS calculation 4. The pin power errors reflect those seen in each of the group fluxes. PSPN agrees well with WIMS, but the diffusion model cannot get the reaction rates correct. On the interface the diffusion solution is partially improved by the use of correction factors.

bulk of the material is not captured accurately by diffusion theory, with the pincell correction factors having almost no impact. The error on the interface is somewhat alleviated by the correction factors, but in all cases is $\ll 1\%$.

The useful information to be extracted from these tests is that:

1. the cross-sections can be accurately transferred from WIMS to PSPN;
2. PSPN is capable of computing a full transport solution in slab geometry;
3. it is more important to capture the thermal flux correctly for this type of interface;
4. very low numbers of angular moments are required to do this.

In addition to this, the improvements due to the use of the SP_N equations might not be significant for a MOX-UOX interface. There is a potential to find improvements in problems where there is an enrichment change between assemblies leading to a large general flux tilt.

In the next section the full assembly geometry will be considered. As has been mentioned, the use of correction factors, in order to preserve the partial currents, was chosen to give an idea of the impact of the homogenisation procedure. It is not practical to perform this process when analysing realistic problems with an array of 81 pincells. The amount of extra data which would be produced by using full GET would be prohibitive. In practice SuPerHomogénéisation (SPH) factors are used to provide preservation of pintype averaged reference reaction rates and leakages. This is because only one correction factor is required per pintype and group, much the same as in full assembly homogenisation.

6.2 Single Assembly Calculations

In this section the computation of the SPH factors is described, and the results of applying them in a SA ILC presented. An advantage of integrating the SP_N nodal method within PANTHER is that the existing framework for calculating the correction factors can be used. In the embedded methodology a set of 6 group homogenised pintype cross-sections and reaction rates are

generated in WIMS and passed to PANTHER. The cross-sections are used in PANTHER ILCs to compute the SPH factors by the non-linear method¹⁴, which can be done for both diffusion and SP_N .

For each pincell type an initial guess of the SPH factors is made. The SPH factor is applied to the within-group SP_N cross-sections in the following way

$$\left[-\mathbf{A} \frac{\partial}{\partial x} \frac{\alpha}{\sigma(x)} \frac{\partial}{\partial x} + \alpha \sigma(x) \mathbf{I} \right] \frac{\boldsymbol{\psi}(x)}{\alpha} = \mathbf{q}(x), \quad (6.6)$$

where the unknowns are defined as in eq. (2.10) and α is the within-group SPH factor. In PANTHER new cross-sections and diffusion coefficients are defined using the SPH factor as $\tilde{\sigma} = \alpha \sigma$ and the corresponding problem solved. The result of applying this initial set of SPH factors is then compared against the reference pintype fluxes from WIMS and updated factors computed. This procedure is repeated until convergence. SPH factors are implemented for the SP_N equations in this way by both EDF and Grundmann and Mittag²⁷.

This is equivalent to applying the same flux discontinuity factor to all sides of the homogenised pincell albeit with a different definition to that of GET. The solution to this problem still preserves reaction rates, but aims to improve the accuracy of the leakages to adjacent pincells when diffusion theory or SP_N are insufficient. The correction factor can be viewed as performing the same function as in eq. (6.4), but instead of preserving the leakage in one direction it preserves an average partial current on all sides of the pincell.

As mentioned in chapter 1 EDF Energy have set up the KAIST 1A small MOX core with zoning benchmark to test their embedded route. Now that the SP_N nodal method is integrated within PANTHER it is possible to recompute the SPH factors using the new method. Instead of presenting all of the results a representative subset is selected. This consists of the two

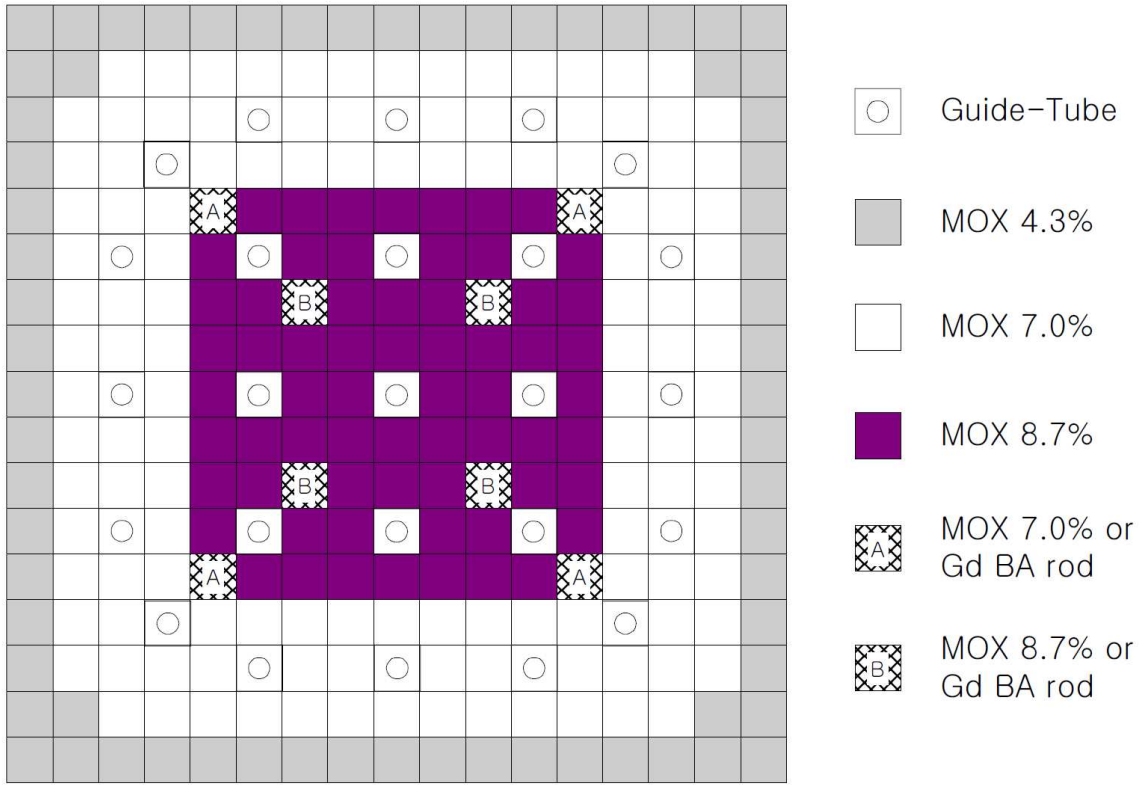


Figure 6.15: The MOX-1 assembly geometry reproduced from the benchmark specification¹. The positions labelled with an A or B represent the locations of the poison pins in assembly MOX-1 (BA_8).

MOX assemblies MOX-1 (BA_8) and MOX-1 which are with and without burnable poison pins respectively. The geometries of the assemblies are displayed in fig. 6.15.

Maps of the pin power errors for the SA ILCs are given in fig. 6.16 and fig. 6.17 for the SP_3 equations with SPH factors applied. The statistics for the pin power errors are given in table 6.2 and table 6.3 for diffusion calculations without SPH factors and diffusion, SP_3 and SP_7 with SPH factors. A clear reduction in the rms, minimum and maximum errors is seen as a result of the application of SPH factors. The most significant improvements are seen in the MOX-1 (BA_8) where the poison pins are present and significant intra-assembly transport theory phenomena are occurring. In fact, with the application of SPH factors, all pin power errors are below 1.2% in assemblies that can have pin power errors as high as 12%. It should also be noted that as a result of the method being incorporated into PANTHER burnup effects

Table 6.2: The pin power error statistics in % for the MOX-1 assembly in the KAIST benchmark. The values with no SPH factors applied have a significantly larger error.

Model	Burnup = 0 GWd/te			Burnup = 20000 GWd/te		
	min	max	rms	min	max	rms
Diffusion no SPH	-0.91	1.19	0.51	-0.47	0.84	0.35
Diffusion	-0.29	0.51	0.14	-0.34	0.43	0.17
SP ₃	-0.61	0.64	0.32	-0.32	0.39	0.16
SP ₇	-0.53	0.54	0.26	-0.26	0.34	0.14

Table 6.3: The pin power error statistics in % for the MOX-1 (BA₈) assembly in the KAIST benchmark. The values with no SPH factors applied have a significantly larger error.

Model	Burnup = 0 GWd/te			Burnup = 20000 GWd/te		
	min	max	rms	min	max	rms
Diffusion no SPH	-1.032	3.411	0.7565	-0.625	1.568	0.4022
Diffusion	-0.325	0.5201	0.1715	-0.9658	1.212	0.2401
SP ₃	-0.6343	0.6599	0.3126	-0.8616	1.11	0.2243
SP ₇	-0.5346	0.6034	0.2585	-0.9849	1.241	0.2202

could be investigated. The last general observation is that the difference in pin power errors is much smaller between diffusion, SP₃ and SP₇ with SPH factors than without SPH factors applied. At the outset this might appear to indicate that there is no improvement as a result of using the SP_N equations. Further analysis is required, however, before this can be concluded.

An important distinction between the corrections defined here and in the line problem must be drawn. In the line problem the SP_N equations are equivalent to the P_N equations and the solution is as accurate as a homogeneous transport calculation. However, in 2D this situation changes significantly. It can be seen in the results above that the SP_N equations definitely do require a correction factor to be applied to properly reproduce the heterogeneous transport solution. This is because in 2D for a pin-by-pin assembly problem the system is not quasi 1D and the SP_N solution is expected to be a poor approximation to the P_N solution, and additionally there are errors from the homogenisation procedure.

In table 6.4 the SPH factors for water holes in the MOX-1 assembly are presented. The size of

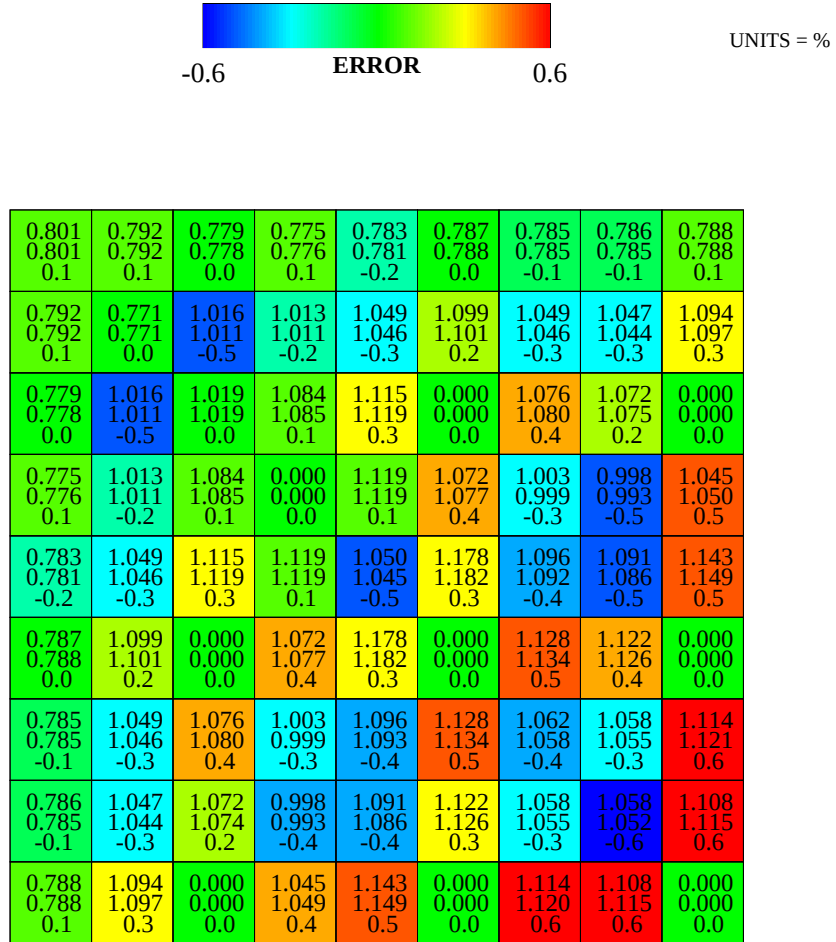


Figure 6.16: Map of the MOX-1 assembly pin power errors. The values in each pincell are reference power, homogenised power and error respectively. These are the SP_3 results of a SA ILC with SPH factors versus WIMS. Only the northwest quadrant is shown due to symmetry.

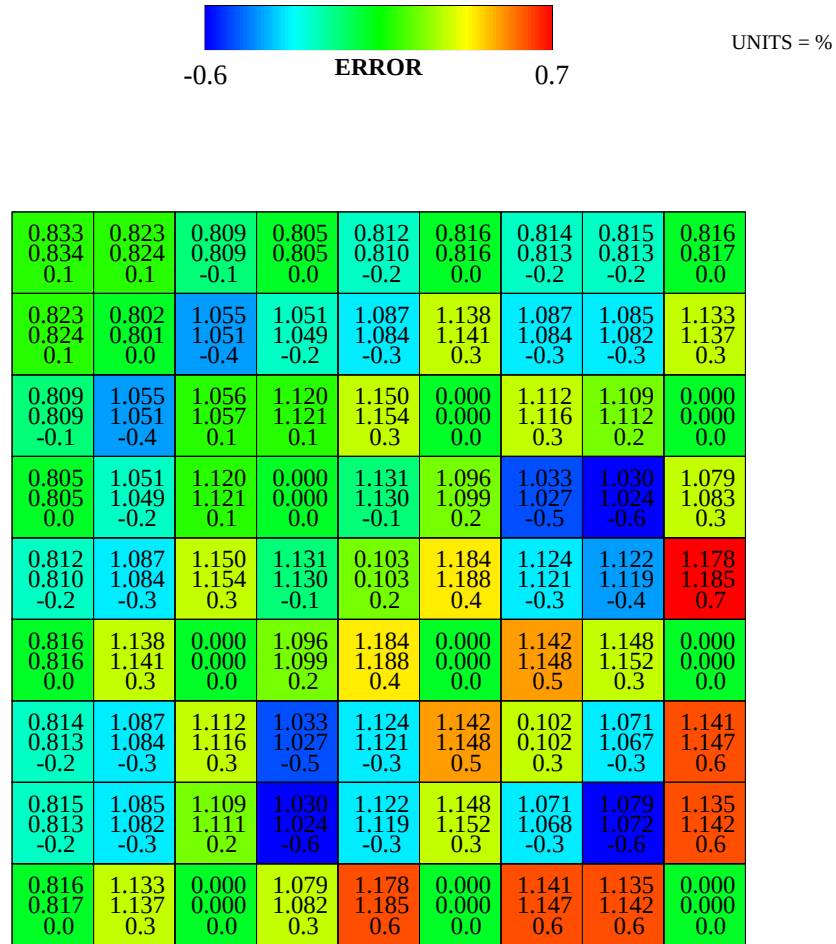


Figure 6.17: Map of the MOX-1 (BA₈) assembly pin power errors. The values in each pincell are reference power, homogenised power and error respectively. These are the SP₃ results of a SA ILC with SPH factors versus WIMS. Only the northwest quadrant is shown due to symmetry.

Table 6.4: The value of the SPH factors for the water holes in the MOX-1 assembly of the KAIST benchmark. The smaller deviation from unity, in the thermal groups, for the SP_N results show that the model is capturing the physics much better.

Model	Energy Group					
	1 (fast)	2	3	4	5	6 (thermal)
Diffusion	0.96533	0.97224	1.02602	1.07238	1.19329	1.18857
SP_3	0.96200	0.97776	1.01672	1.04498	1.10316	1.09817
SP_7	0.96637	0.98598	1.00925	1.02487	1.06081	1.07756

these give some indication of the accuracy of the physical model used to solve a given problem.

A value of unity indicates that the physical model can produce the same results as the lattice cell code. It can be clearly seen that in the thermal range the diffusion theory SPH factors are significantly bigger than those of the SP_N equations. This tells us that the SP_N equations are doing a better job of approximating the true behaviour than the diffusion equation. The other conclusion is that the improvement of the SP_7 over the SP_3 results is much smaller than SP_3 over diffusion. It could be argued looking at table 6.2 and table 6.3 that the increased accuracy of SP_7 over SP_3 is not significant.

6.2.1 Summary

A lot of individual results have been noted in this section and the overall impact of these is commented on here. It appears that it is necessary to use SPH factors to correct for deficiencies in the approximate model in the neighbourhood of water holes, Gd pins and control rods. Applying SPH factors in the SA ILCs brings the errors down to the same level for diffusion, SP_3 and SP_7 models. However, the impact of using the SP_N equations in place of the diffusion equation does have some significance. The actual values of the SPH factors indicate that the SP_N equations are capable of providing a more accurate approximation to the reference solutions as the corrections are smaller than those of the diffusion model. This means that when the SPH factors computed here are applied in colorset and whole core calculations, the

Table 6.5: This table presents the pin power error statistics for the 6 group pin-by-pin calculations using different physical models.

Model	mean	std	rms	min	max
Diffusion	-0.008045	0.7944	0.7944	-1.906	1.536
SP ₃	0.06728	1.136	1.138	-3.069	1.79
SP ₅	0.07113	1.154	1.156	-3.194	1.703

benefits of using the SP_N equations may be seen.

6.3 Colorset Reproduction

In the previous section a set of pin type SPH factors have been computed using the results from SA ILC calculations. The intention is that the SPH factors will correct the transport effects which cannot be captured by a lower-order model even in an environment significantly different from that in which they were computed. These pintype SPH factors are now applied to one of the 6 group pin-by-pin colorset calculations that form part of the embedded methodology.

6.3.1 6 Group Pin-by-Pin Results

The solutions to the 6 group pin-by-pin colorset calculations used to define the corrections to the 2 group colorset calculation in the embedded methodology are now considered. This is done to quantify how well the different physical models capture the interface effects. The diffusion results are shown in fig. 6.18 and the SP₃ results in fig. 6.19. The corresponding pin power statistics are given in table 6.5.

It can be seen that the diffusion results are nominally better than those from the SP₃ calculation. The interesting result with respect to the SP_N nodal method is the difference between the diffusion and SP₃ results. There appears to be an error limiting the accuracy in the 6 group

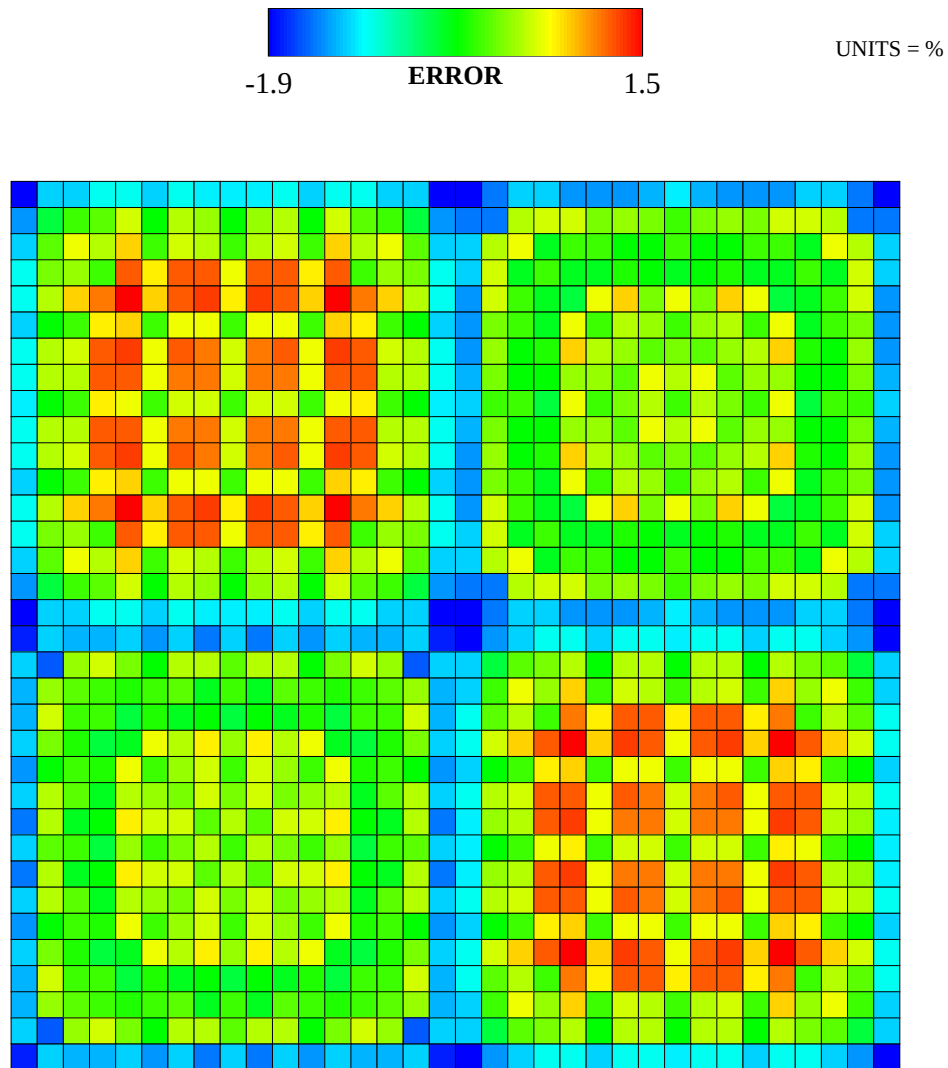


Figure 6.18: This map shows the pin power errors in a 6 group pin-by-pin diffusion calculation of the MOX-UOX colorset with pintype SPH factors applied.

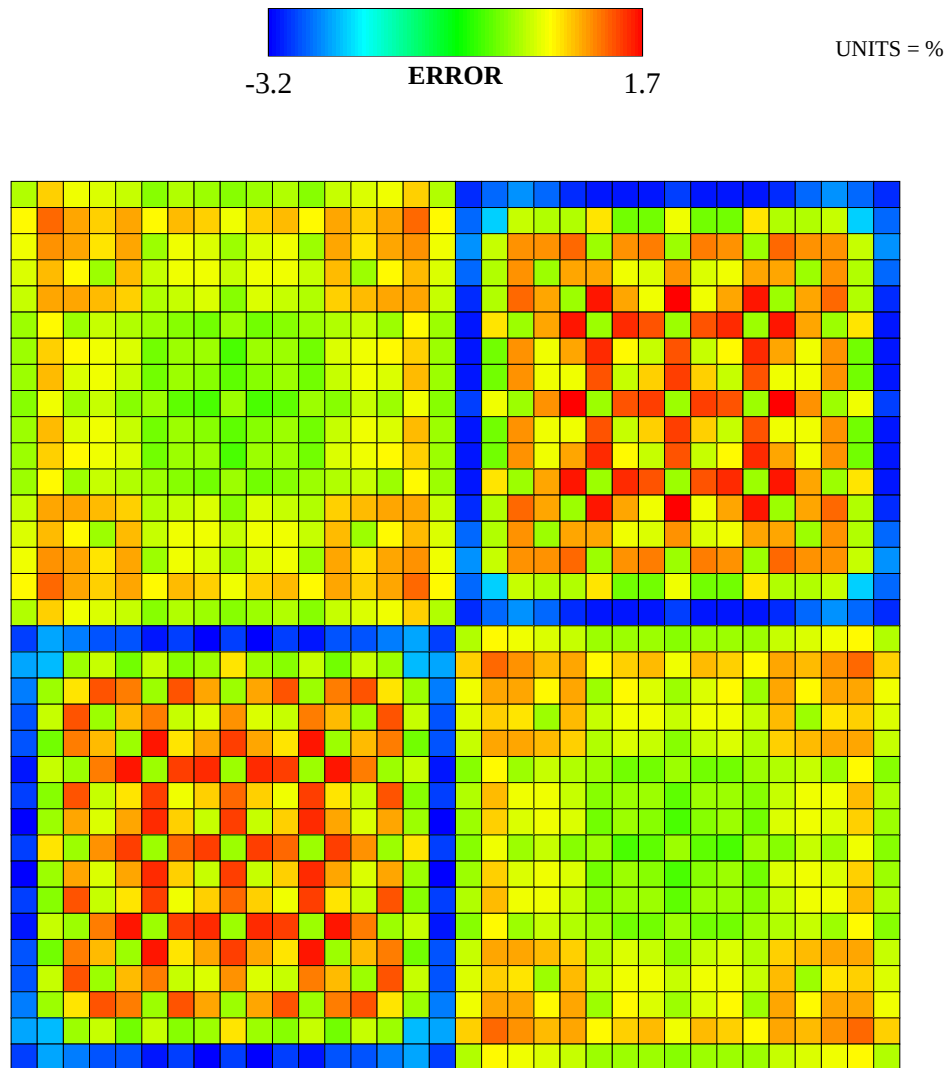


Figure 6.19: This map shows the pin power errors in a 6 group pin-by-pin SP_3 calculation of the MOX-UOX colorset with pintype SPH factors applied.

pin-by-pin colorset that is larger than the difference between diffusion and the approximate transport method. This is to be expected considering the results of the line of pincells and single assembly results. In these situations both methods showed an error due to the homogenisation process of $\approx 2\%$.

The largest errors seem to occur at the periphery of an assembly and seem to be similar away from the corners. This provides confirmation that the line of pincells is a good model problem in which to study the effects of homogenisation. The general trend shows that in all cases the largest errors arise from the effects occurring at the edges of the assembly. The existing techniques capture intra-assembly effects well.

6.3.2 Applying the Embedded Methodology to a Simple Colorset

In order to compute the solutions presented in this section the embedded methodology has been applied to a colorset problem. This entails the computation of SPH factors for each assembly in a SA ILC and their application in conjunction with the 6 group material data in a calculation identical to that presented in the previous section. The results from this 6 group pin-by-pin calculation are then compared against a solution to the 2 group homogenised assembly version of the colorset. This is done to compute corrections to the 2 group homogenised cross-sections, discontinuity factors and pin power form factors such that the solution of the 6 group pin-by-pin colorset can be reproduced from the 2 group calculation. Essentially GET is applied with the higher-order solution being 6 group pin-by-pin and the lower-order an assembly homogenised 2 group diffusion calculation.

The solution to the colorset is then computed using diffusion theory in 2 groups with homogenised assembly data and the 6 group corrections applied. The pin powers are reconstructed

Table 6.6: The pin power error statistics from the embedded methodology applied to a colorset calculation with corrections computed using different physical models.

Model	mean	std	rms	min	max
Diffusion	0.2554	1.988	2.005	-4.876	6.298
Diffusion Corrected	-0.07699	0.8552	0.8586	-2.757	1.074
SP ₃ Corrected	0.003412	0.9878	0.9878	-2.532	1.521
SP ₅ Corrected	0.01182	1.005	1.005	-2.696	1.421

and compared against a 6 group heterogeneous WIMS model of the colorset to see how well they have been reproduced. The results of using the embedded methodology with diffusion theory in the 6 group problem are shown in fig. 6.20 and the results of using SP₃ in the 6 group problem are shown in fig. 6.21. The results of using the standard 2 group diffusion calculation scheme are shown in fig. 6.22 to give an idea of the initial errors observed.

The results show clearly that the error is significantly reduced with the use of the embedded methodology regardless of the underlying physical model chosen. The pin power statistics tell us relevant information about the improvements and are given in table 6.6. The rms error is changed from an initial value of 2% to the improved values of 0.86% and 0.99% for the diffusion and SP₃ models respectively. The maximum (absolute) pin power error is also reduced from 6.3% to 2.8% and 2.5% for the diffusion and SP₃ models respectively. This represents a reduction by half of the peak pin power errors.

As in the 6 group pin-by-pin calculation the largest errors are on the periphery of the assemblies and intra-assembly effects are captured well. The error limiting the accuracy of the embedded method is still larger than the difference between diffusion and the approximate transport method. In summary the embedded methodology can reduce by more than half the errors in the standard 2 group SA approach.

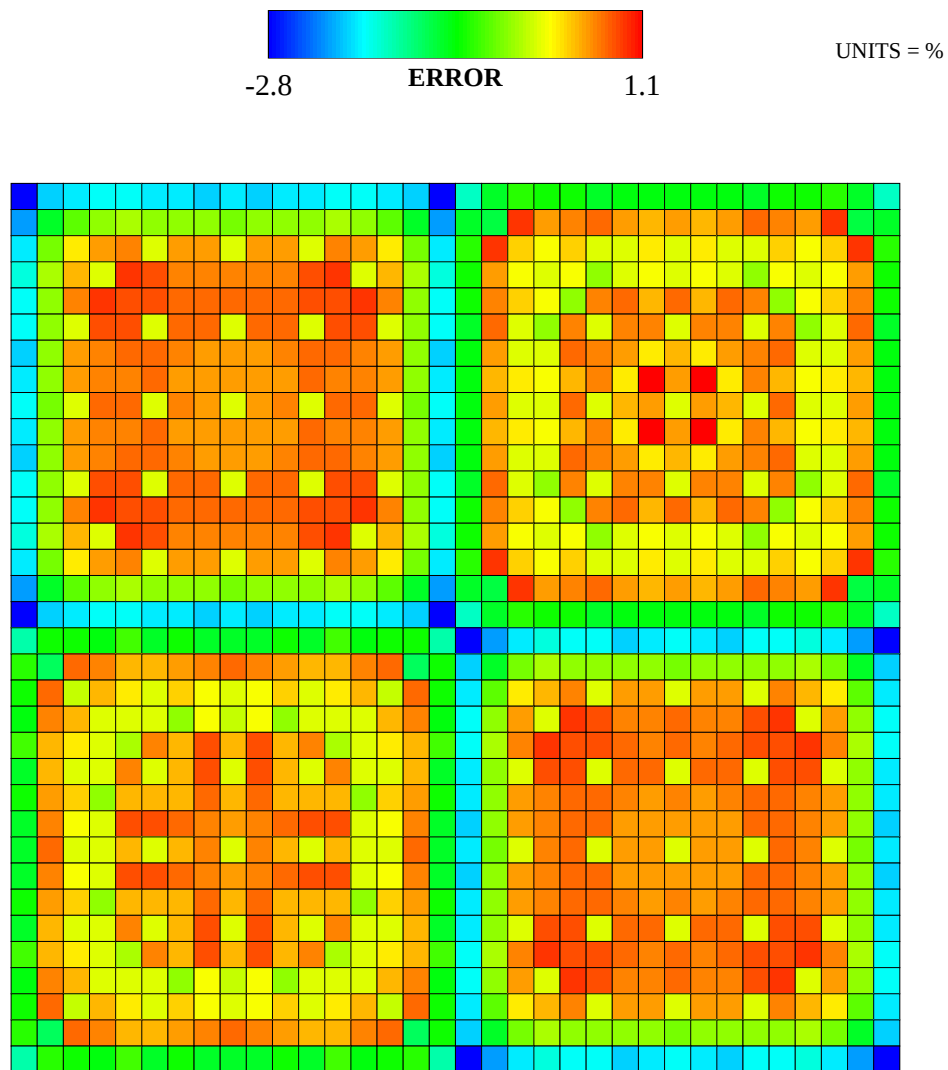


Figure 6.20: This map shows the pin power errors from applying the embedded methodology using the diffusion equation.

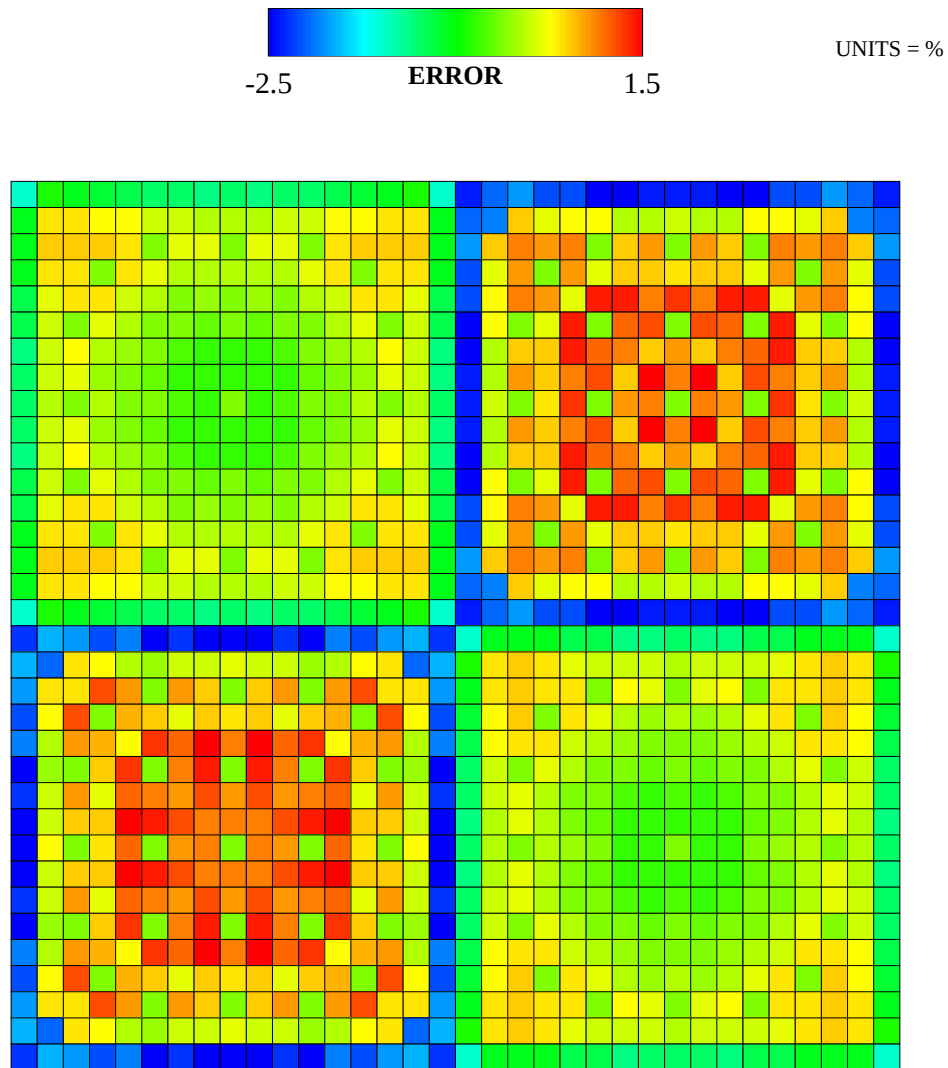


Figure 6.21: This map shows the pin power errors from applying the embedded methodology using the SP_3 equations.

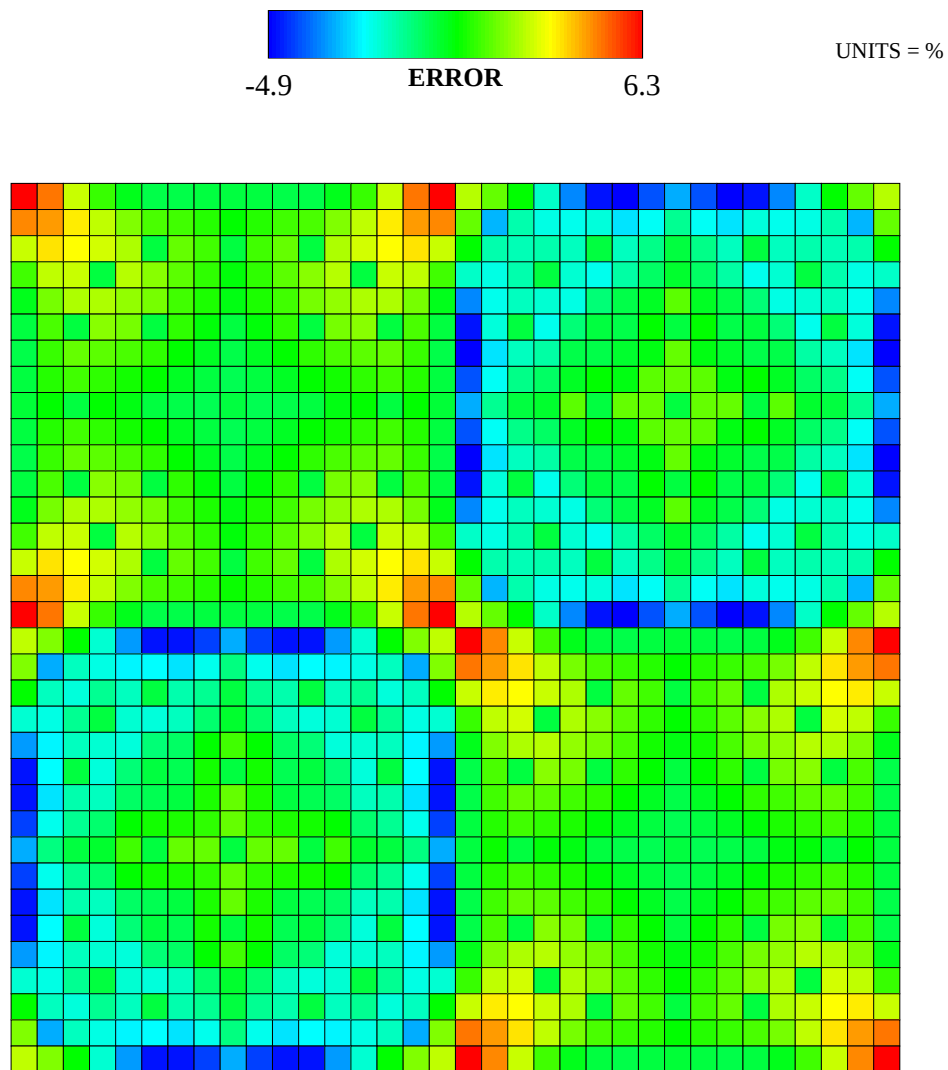


Figure 6.22: This map shows the pin power errors from applying the standard calculational route to a MOX-UOX colorset.

6.4 Application to the KAIST Benchmark

In the previous sections the groundwork has been laid down for the application of the SP_N nodal method to realistic reactor core problems. In order to test the capabilities of the embedded method with an integrated SP_N capability the KAIST 1A small MOX core with zoning benchmark was solved. The geometry has been given previously in fig. 1.2 and the problem was solved with the control rods out.

The embedded methodology was designed and implemented in PANTHER using the existing diffusion nodal method and applied to the KAIST benchmark. What the results in this section represent are the computation of a solution to the same problem, but using the SP_N nodal method in the embedded 6 group pin-by-pin calculation instead. It is a substantial test of the success of integrating the SP_N nodal method into the existing PANTHER framework. All of the SA calculations have been redone to define SPH factors for the SP_N equations and the reflector data has also been recomputed to be consistent. The embedded colorsets can then be solved with SPH corrected SP_N and the main calculational route is not changed. The corrections from the embedded methodology with the SP_N nodal method can be applied to the 2 group whole core calculations even during burnup.

The error in the reconstructed pin powers compared against a WIMS reference are illustrated in figs. 6.23 to 6.25 which are computed using: the standard calculational route, the embedded method with diffusion and the embedded method with SP_3 respectively. It can be seen from these results that the embedded diffusion method results are slightly better than the embedded SP_3 results. It should be said, however, that the large negative errors in the SP_3 solution are seen only in low power pins immediately next to the reflector which are $\approx 10\%$ of the largest pin power. The accuracy on the most important (high power) pins is of a similar size. The

Table 6.7: This table presents the pin power error statistics for the embedded methodology applied to the full KAIST benchmark using different physical models.

Model	mean	std	rms	min	max
Diffusion	-0.54	2.74	2.80	-11.54	5.90
Diffusion corrected	-0.15	0.83	0.85	-3.47	3.27
SP ₃ corrected	0.10	1.07	1.08	-5.45	2.95
SP ₃ 20 GWd/te	0.05	0.75	0.75	-5.85	8.94

most important result is that both the diffusion and SP₃ embedded methods are significantly better than the traditional calculational route. This can be confirmed by looking at the pin power error statistics in table 6.7.

The results using the embedded SP₃ method after 20 GWd/te of burnup are shown in fig. 6.26 and the statistics in table 6.7. Again the large errors are only present in very low power pins, and in fact the solution after burnup is more accurate than at the Beginning Of Life (BOL). This result shows that the SP_N nodal method is capable of performing practical core calculations as part of the embedded method. No extra work had to be performed to get the burnup calculations to work. Once the corrections to the 2 group data from the 6 group colorset SP₃ calculations have been defined, then the burnup calculations proceed as in the standard calculational route. The corrections for a given loading pattern have all been computed offline before the full core analysis with burnup is performed.

6.5 Summary

In this chapter the results of a series of problems of increasing complexity have been presented. The first problem is a line of 10 MOX and 10 UOX pincells, which when homogenised represent a slab geometry problem. This is representative of the interfaces seen between assemblies in a reactor loaded with MOX. The MOX pins were 8.7% enriched and the UOX 3.3%. It was found that in this simple setting the homogeneous data with correction factors produce solutions of

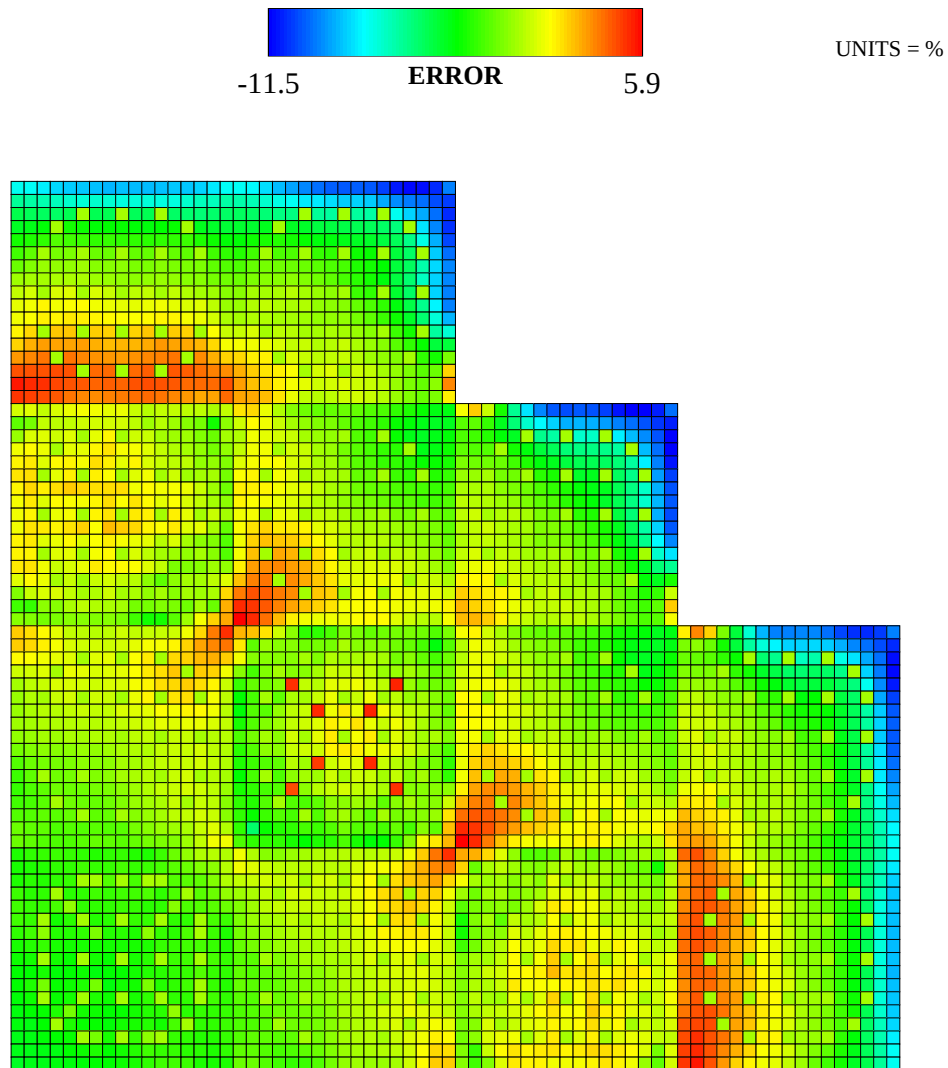


Figure 6.23: The reconstructed pin power errors for the full KAIST benchmark using the standard calculational route.

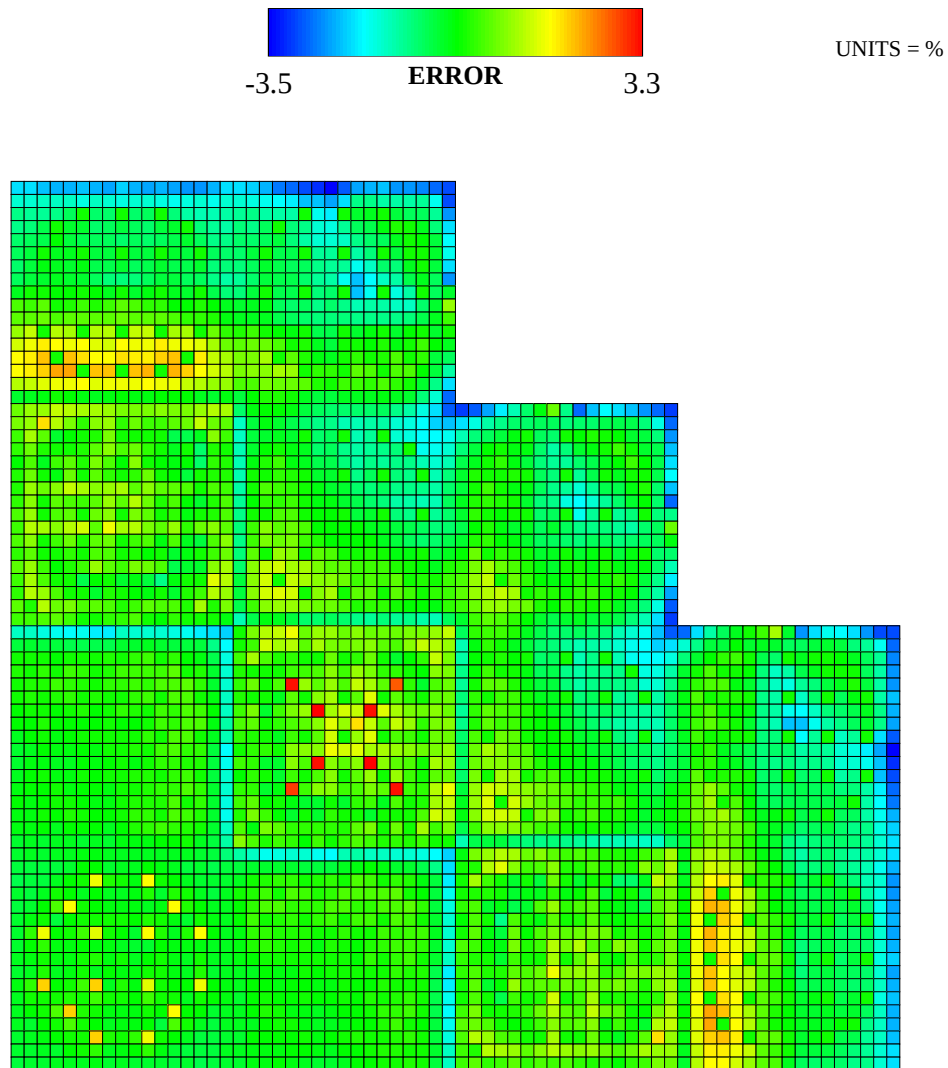


Figure 6.24: The reconstructed pin power errors for the full KAIST benchmark using the embedded methodology and a diffusion solver.

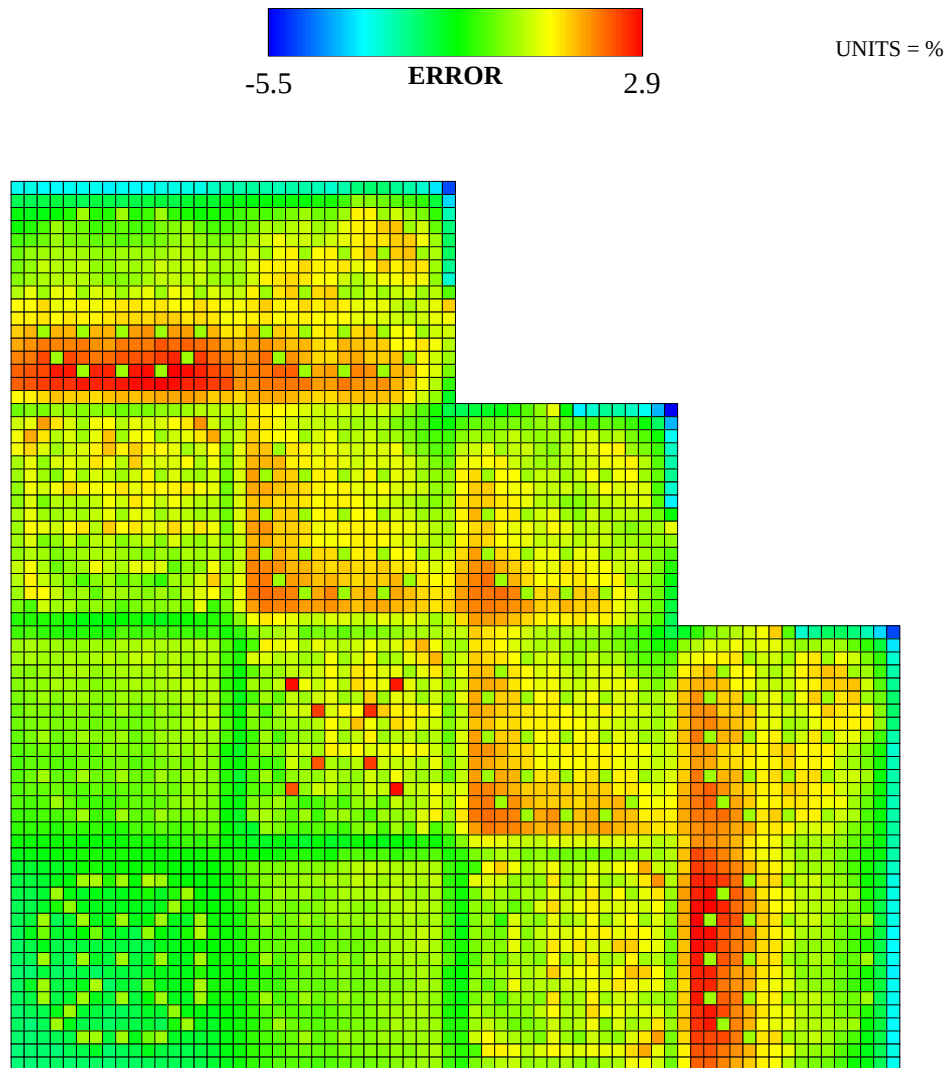


Figure 6.25: The reconstructed pin power errors for the full KAIST benchmark using the embedded methodology and an SP_3 solver.

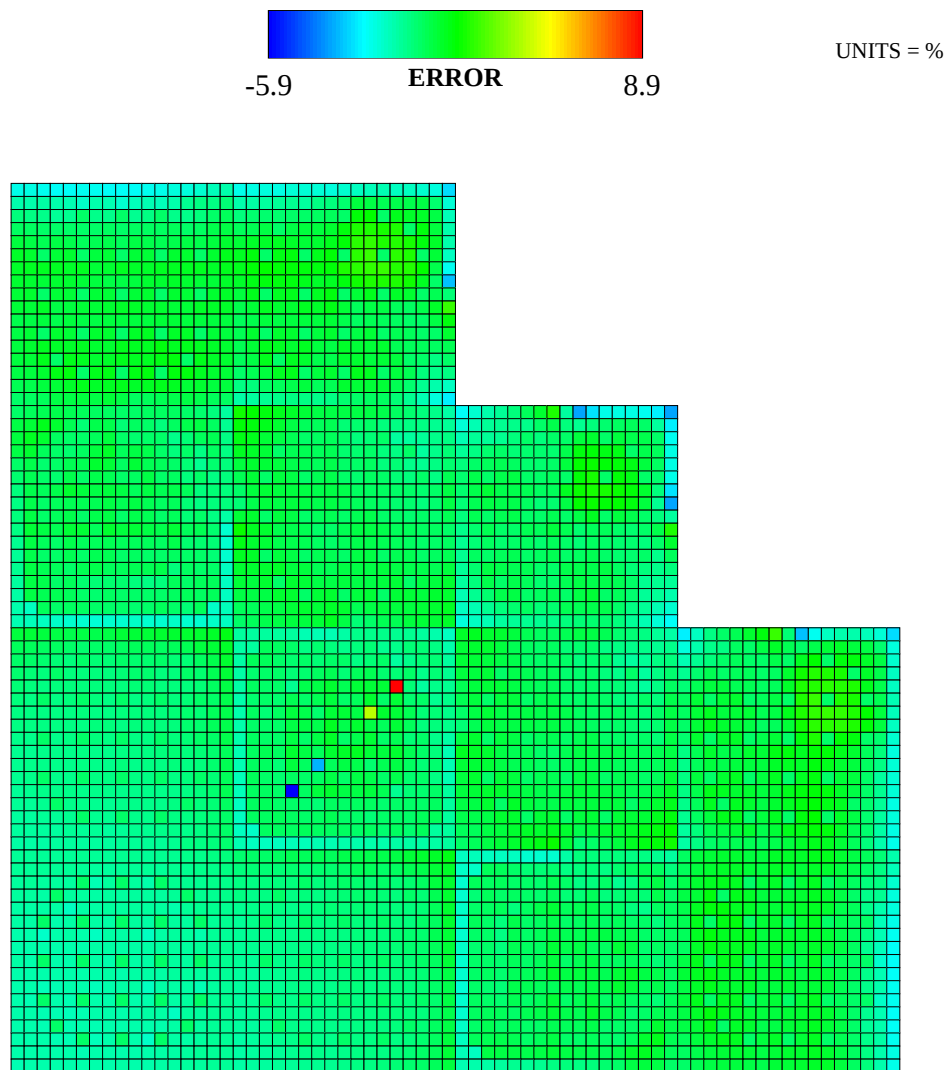


Figure 6.26: The results of using the embedded methodology with an SP_3 solver for 20 GWd/te of burnup.

equal accuracy for both the diffusion and SP_3 equations. Further, the improvements of SP_5 and SP_7 over SP_3 are negligible.

The use of pincell correction factors for the diffusion equation is found to be significantly more accurate than using the homogeneous material data without them. This is in spite of the fact that the correction factors are derived in a situation that is not entirely representative of that on the interface in the line of pincells. The SP_N equations are not found to need the correction factors in this setting, and applying them does not significantly impact the error in the solution.

For the case of UOX pincells with a change of enrichment the use of the SP_N nodal method corrects almost all of the error. In contrast to a MOX-UOX interface the majority of the error is in the bulk of the material. The pincell correction factors are almost unity and therefore have little impact on the final solution. This indicates that the error seen here in the diffusion solution is purely attributable to transport effects which are captured successfully by the SP_N equations. There is a $<1\%$ interface error from homogenisation that cannot be removed by using transport theory.

The solution to the line of pincells indicated that the pin powers, the main quantity of interest, were sensitive to only the thermal flux. It also indicated that the use of any physical model with the existing homogenisation techniques cannot get rid of all of the error in the solution. In fact, the improvement from using the transport solver instead of the diffusion solver was not significant.

In order to model realistic problems, full assemblies need to be homogenised and correction factors defined. Due to practical constraints relating to the amount of data and the information that can be extracted from WIMS, the SPH method was chosen to define correction factors and the results agreed well with the published literature. The corrections were most effective on assemblies that contained Gadolinium pins where it is expected significant transport effects

are present. The error was reduced on the gadolinium pin powers from 12% to $\approx 1\%$. The application of SPH factors to a SA ILC produced similar levels of accuracy for both diffusion and SP_3 models as was indicated in the line of pincells. The main difference was in the size of the correction factors. The corrections for the diffusion model were significantly larger than those for the SP_3 model. This indicates that the SP_N equations produce a better approximation to the transport solution than the diffusion equations.

A colorset calculation was then performed to test the impact of the different physical models on the embedded methodology. First the 6 group pin-by-pin model was considered as the solution to this problem is used to derive the corrections to the standard 2 group data. The solutions to the 6 group pin-by-pin model showed that the SP_N and diffusion models were capable of achieving similar accuracy. The results show that the main error is at the interface of the assemblies which have had their data derived in isolation. This is expected from the analysis of the line of pincells.

The embedded methodology was then applied to the colorset calculation using the corrections defined in the 6 group pin-by-pin model. The results were much the same as for the explicit 6 group pin-by-pin solution. The largest errors were seen on the interface and intra-assembly effects were captured well. The diffusion and SP_N equations used within the embedded methodology were shown to achieve the same accuracy with a residual error from the homogenisation procedure.

The last calculation was of the full quarter core in the KAIST benchmark. The results displayed are reconstructed pin powers for the whole region. The conclusions are the same as in the colorset calculations. There were some higher error pin powers when the SP_N equations are used, but these are all on low power pins and are of no real concern. Overall the pin power errors are halved when using the embedded methodology with both physical models.

All of the results in this section point to a clear conclusion for the embedded methodology. With the existing homogenisation techniques and data provided by WIMS there is no advantage to using the SP_N equations over the diffusion equation. Most of the error appears to arise from an insufficient number of energy groups which is addressed by the embedded method. The residual homogenisation error, which has some spectral and spatial aspects, could only be removed by the implementation of a superior homogenisation technique.

The integration of the SP_N nodal method in the embedded methodology within PANTHER is highlighted with the production of a pin power error map after 20GWd/te of burnup. This shows that the procedure is accurate, even with the new solver, and that after burnup the solution has increased accuracy.

Chapter 7

Conclusions

In this chapter the main conclusions of the research contained in this thesis are summarised to give a global view of what has been achieved. The research objectives were to create an SP_N nodal method, integrate this into the embedded methodology developed by EDF Energy and quantify the accuracy resulting from using an approximate transport model for problems involving advanced fuels. All of these objectives have been achieved; however, potential improvements were identified during the course of the research. To this end, suggestions for further research are made at the end of this chapter.

This thesis starts with an analysis of the SP_N equations resulting in two transformations that allow a nodal method to be applied. In the literature there exist both an *ad hoc* algebraic and, more fundamentally, a similarity transformation to do this. The algebraic method has previously only been applied to the SP_3 equations and in this thesis it was extended to the SP_N equations. This type of transformation has a downside in that it results in negative values for cross-sections in the transformed system. This was shown to produce problems with convergence and required the use of more advanced, and therefore computationally expensive, solvers.

It is believed that this thesis represents the first time that the similarity transformation has been used for a nodal method. It has been used previously to solve the SP_N equations using other numerical methods, but it is crucial in the application of a nodal method. This is because it removes the angular coupling from the derivative term in the SP_N equations. It was then proved that the cross-sections in the abstract space, defined by a similarity transformation, are all positive. This means that *any* multi-group diffusion solver should be capable of solving this set of equations to determine the SP_N solution. The author believes that the proof that the cross-sections are positive is a new result.

The analysis was taken a step further to investigate the implementation of vacuum boundary conditions. Mark boundary conditions were derived as in the literature and it was determined that they can be applied in a multi-group diffusion code that has the capability of applying an albedo boundary. The Marshak boundary conditions were also derived for the abstract space which is a new result to the knowledge of the author. This cannot, however, be implemented in a multi-group diffusion solver without significant changes as it couples all of the angular moments at the boundary.

It was decided that a Semi-Analytic Nodal Method (SANM) should be used to provide solutions to the SP_N equations. The specific implementation was taken directly from the literature to show that a standard nodal diffusion solver can be used with the transformed SP_N equations. The solver was initially written for and tested on multi-group diffusion problems. An extra subroutine was then added to transform a set of diffusion cross-sections into those for the SP_N equations. This augmented problem was solved using the nodal diffusion solver and the solution transformed back into the physical space and only the scalar flux retained.

To efficiently solve whole core problems a Coarse Mesh Finite Difference (CMFD) method is usually employed. This is to reduce the memory requirements and accelerate the convergence

of the nodal method. It has been found that the algebraic transformation produced a set of equations that could not be solved by the standard CMFD methods, and for this reason a version with a better theoretical background was chosen. The Effective Diffusion Coefficients (EDCs) were employed to implement the CMFD method as they should provide greater stability. The EDCs have only been derived for the Analytic Nodal Method (ANM) and to the author's knowledge this is the first time it has been done for the SANM. Further, it is believed this is the first time the EDCs have been applied to accelerate an SP_N nodal solver. It was also found that the EDCs can reduce the total number of power iterations required to solve problems with a coarse mesh.

Unfortunately even the improved stability of the EDCs was not enough to ensure that the algebraic transformation would converge. The situation is completely different, however, for the similarity transformation. Due to the proven properties of the cross-sections the solver converged for all types of CMFD method. This confirms that the similarity transformed version of the SP_N equations has the same properties as the multi-group diffusion equation with respect to the solvers used. Although a nodal method has been developed previously that can solve the SP_N equations, it involved an approximation of the angular coupling and solved a different form of the equations. This method involves no such approximation and therefore should be capable of computing more accurate solutions.

The SP_N nodal method was integrated into the Pwr and Agr Neutronics and Thermal Hydraulics Evaluation Route (PANTHER) package so that the existing geometry and data generation capabilities could be used, and the solver could be used in the embedded methodology. This step also made it possible to re-run existing benchmarks in PANTHER using the new solver and easily set up new ones. A comprehensive set of benchmarks were performed as verification for the new solver. This included diffusion problems to test that existing results could

be reproduced, and also small cores with vacuum boundaries to test the approximate transport and vacuum boundary capabilities. The success of the SP_N nodal method in these benchmark cases confirms the assertions made when developing the theory in earlier chapters. It has been made clear that the similarity transformation of the SP_N equations is much more appropriate for a nodal method.

After the SP_N nodal method was integrated into PANTHER the effects of using it in the embedded methodology were investigated. A series of preliminary calculations were performed to determine the impact of homogenisation on a simple representative problem. This was a line of 10 Mixed OXide (MOX) and 10 Uranium OXide (UOX) pincells, which when homogenised becomes a slab geometry problem. This is representative of the interfaces seen between assemblies in a reactor loaded with MOX. The solution to this problem indicated that the diffusion and SP_N solutions did not differ significantly, but that pincell correction factors were required for effective homogenisation of the diffusion equation. These pincell correction factors improved the solution even when they were derived in an environment significantly different from that in which they were applied. The SP_N equations did not require pincell correction factors, and their application did not decrease the error. For both the diffusion and SP_N equations a residual error of $\approx 1\%$ was seen at the interface, which was attributed to the homogenisation procedure.

Using an identical approach a second line of pincells was modelled, but in this case both types of pincell were UOX with different enrichments. This problem represents a situation in which there is significant leakage from one area into another. In this case the majority of the errors were seen with diffusion and occur in the bulk of the material away from the interface. The SP_N equations had almost no error in the bulk and similar error on the interface. The pincell correction factors were very close to unity meaning that in this problem they have little impact on the solution. What is being observed here is a purely transport effect being corrected for by

the SP_N solver.

In 2D it is not practical to use the same pincell correction factors and the pintype SuPerHomogénéisation (SPH) factors were used instead. These are computed using a Single Assembly (SA) Infinite Lattice Calculation (ILC) in PANTHER and are necessary to correct the SP_N and diffusion methods for transport phenomena. It was again found that the performance of diffusion and SP_N are similar, but in 2D both require pintype correction factors. The maximum pin power errors were found to be $\approx 1\%$ for both physical models with pintype SPH factors applied. The pintype correction factors were applied in the same way as in the literature and yielded similar results.

Once the pintype SPH factors have been computed for the SA cases these can then be used in the 6 group pin-by-pin colorset calculations in the embedded methodology to provide an accurate solution from which SA correction factors can be derived for the 2 group homogeneous data. The embedded methodology was tested on a colorset consisting of 2 MOX and 2 UOX quarter assemblies. The results showed the diffusion and SP_N equations achieve similar accuracy, and both are significantly better than the standard calculational route reducing the pin power errors by $\approx 50\%$.

To highlight the benefits of integrating the SP_N nodal method within PANTHER the full quarter core from the KAIST benchmark has been solved using the embedded methodology. The pin powers have been reconstructed and the embedded method shows improved accuracy over the standard route with the errors reduced by $\approx 50\%$. This figure is slightly misleading as the largest errors in the SP_N results, from the embedded methodology, are on low power pins which are of little interest to the practitioner. The reduction in the pin power error for the high power pins is greater than this. The SP_N equations again achieved similar accuracy to the diffusion equation for the pin powers in the KAIST quarter core. The burnup calculation

was performed until 20 GWd/te and showed that the accuracy of the embedded method holds through burnup even with the SP_N nodal method.

It has been concluded that the SP_N nodal method has been successfully integrated into the PANTHER package. The embedded methodology was applied to a full quarter core with burnup and produced a significant increase in accuracy over the standard route. There does, however, appear to be no advantage to solving the SP_N equations over the diffusion equations in the embedded methodology. There is a residual error arising from the homogenisation procedure, and this is larger than any improvements resulting from the use of the SP_N equations. It is suggested that the homogenisation procedure needs to be improved in order to obtain a more accurate solution. The small difference between the diffusion and SP_N solutions indicates that the errors in the standard route are dominated by spectral effects, which are effectively captured by the inclusion of more energy groups in the embedded methodology.

During the course of performing the research contained in this thesis certain questions arose relating to the methods used. These could not be addressed during the course of this research, and in the next section some suggestions for further research are made based on these observations.

7.1 Future Research Directions

The future research directions are split into two themes. The first relates to the SP_N nodal solver as a standalone numerical method for solving approximate neutron transport problems. The second theme outlines possible extensions to the embedded methodology taking into account the observations described in this thesis.

7.1.1 Improvements to the SP_N Nodal Method

The SP_N nodal method has been benchmarked and shown to achieve the expected accuracy of a method of this type, and this is therefore not a concern. The main perceived weakness of the implementation in this thesis is the execution speed. The execution speed for the SP_N nodal method applied to the Takeda benchmark model 1 case 2 is shown in fig. 7.1. The multiplication factor gives information about how much longer an SP_N calculation takes than the corresponding diffusion one. The interesting thing to note is the size of the multiplication factor when going from SP_1 to SP_3 as this represents the largest decrease in error. The execution times of the code for the SP_1 calculation in both the physical and the abstract space are almost identical. This tells us the large initial increase is not due to the similarity transformation of the cross-sections leading to a system of equations that is harder to solve. It means the increase in solution time is just a result of the system getting larger, and this would be observed even in an optimised neutron diffusion code.

It has been noted that the increase in the number of groups challenges the ANM and this has been found in the SANM due to the need to resolve the group-to-group interactions. At every power iteration and interface in the core there is a matrix system which needs solving of order groups x moments. A direct solver is used for this, which can prove to be slow for large numbers of groups. One method to circumvent this in the SANM is to replace the direct method with an iterative one which has been attempted by Kim et al.⁶¹ with some success.

Although some improvements are made by implementing the CMFD method it may not be enough. At some point a global finite difference system of equations with groups x moments equations needs to be solved. This can be reduced by defining a CMFD method which takes a local groups x moments solution and defines 2 group diffusion parameters on the global scale.

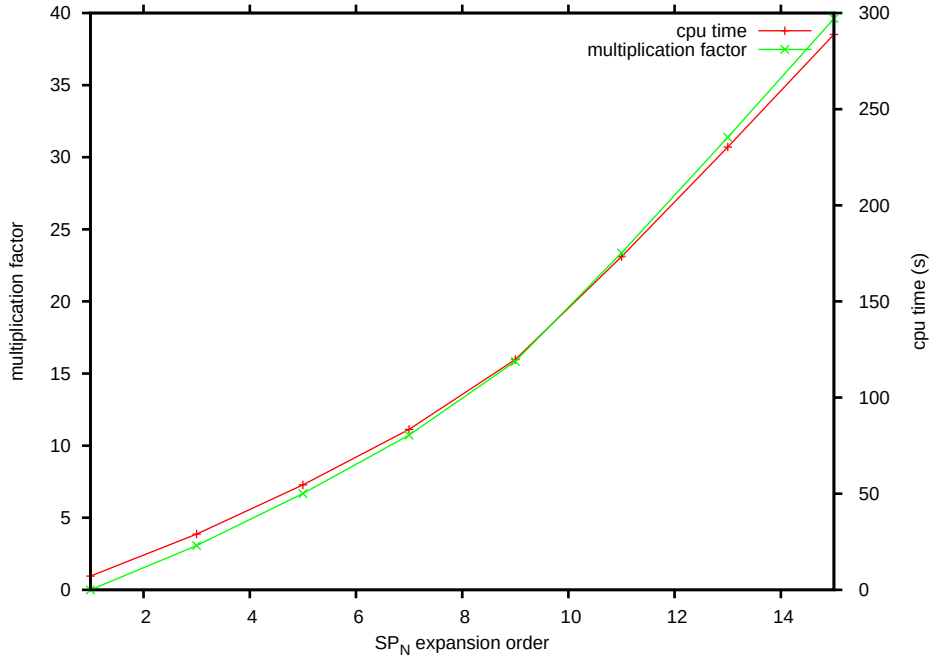


Figure 7.1: A graph showing the execution times of the SP_N nodal method when applied to the Takeda benchmark model 1 case 2. The multiplication factor is the amount by which the time differs from the previous (smaller) number of moments. Interestingly there is an increase of time of about 4 times when going from SP_1 to SP_3 . Otherwise each doubling in the number of “groups” results in the execution time increasing by less than a factor of 2.

This has also been implemented in another setting with some success by Lewis¹², Yoon and Joo⁶³.

7.1.2 Improvements to the Embedded Methodology

In the embedded methodology an initial line of pincells was considered to investigate the effect of the homogenisation procedure on the solution at a MOX-UOX interface. It was seen here that the homogenisation procedure used can correct some of the effects, but a small error of $\approx 1\%$ remains. It is postulated that this contains residual spectral effects and also effects due to the underlying heterogeneous geometry. What is then observed in 2D is just the compounded effects of these residual errors. It is therefore advantageous to focus effort on improving the solution to the line problem as any increase in accuracy there should carry through to the whole core.

In order to improve the homogenisation procedure a lot of extra work is required. Corrections will be needed for the higher-order angular moments of the SP_N equations. The work of Sanchez⁹ could be implemented, although this requires a lattice cell code which can compute the spherical harmonics expansion coefficients of the angular flux. This should begin to give an upper bound to the question of how much the solution can be improved when the material data is derived in SA ILCs.

Once an idea of this has been obtained then the question of the best way to bring local information about the core environment into the SA or colorset calculations can be answered. Once we are iterating from whole core to SA are colorsets even needed? How much more expensive is this procedure, and are the increases in accuracy more or less than a better homogenisation procedure? Do you in fact need both to obtain a more accurate solution?

Another question that has not been addressed is the impact of using the SP_N nodal method on the whole core with assembly homogenised regions. One of the developments in SIMULATE-5²¹ is a sub-model which computes an SP_3 solution to a full 2D horizontal slice through the core. This is to correctly model the flow of neutrons around the reactor which cannot be captured by diffusion theory. In order to do this the homogenisation procedure must be adapted to work with the SP_3 equations.

Appendix A

The Normalised Legendre Polynomials

The normalised Legendre polynomials are defined by:

$$p_n(\mu) = \sqrt{\frac{2n+1}{2}} \bar{p}_n(\mu), \quad (\text{A.1})$$

where $\bar{p}_n(\mu)$ is the Legendre polynomial of order n . The orthogonality relationship is then:

$$\int_{-1}^1 p_n(\mu) p_m(\mu) d\mu = \delta_{nm}, \quad (\text{A.2})$$

where δ_{nm} is the Kronecker delta. This definition can be used to write down the normalised Legendre polynomials:

$$p_0(\mu) = \frac{1}{\sqrt{2}}; \quad (\text{A.3})$$

$$p_1(\mu) = \sqrt{\frac{3}{2}}\mu; \quad (\text{A.4})$$

$$p_{n+1}(\mu) = \frac{(2n+3)^{1/2}}{n+1} \left[(2n+1)^{1/2} \mu p_n(\mu) - \frac{n}{(2n-1)^{1/2}} p_{n-1}(\mu) \right]. \quad (\text{A.5})$$

The last relationship, between the normalised Legendre polynomials, that is needed to derive the P_N equations in slab geometry is the addition theorem. This theorem is stated in terms of the spherical harmonics and in 1D reduces to:

$$p_n(\mu \cdot \mu') = \sqrt{\frac{2}{2n+1}} p_n(\mu) p_n(\mu'). \quad (\text{A.6})$$

A.1 Eigenvalues and Eigenvectors of Coupling Matrix

Consider the coupling matrix $\mathbf{A}$ from the even-parity slab geometry neutron transport equation. It is computed from the expression

$$\mathbf{A} = \int d\mu \mathbf{p}(\mu) \mu^2 \mathbf{p}^T(\mu). \quad (\text{A.7})$$

In order to perform this integral the recurrence relation is used twice giving

$$\begin{aligned} \mu^2 p_n(\mu) = \frac{1}{(2n+1)^{1/2}} \left[\frac{n+1}{2n+3} \left(p_n(\mu) \frac{n+1}{(2n+1)^{1/2}} + p_{n+2}(\mu) \frac{n+2}{(2n+5)^{1/2}} \right) \right. \\ \left. + \frac{n}{2n-1} \left(p_{n-2}(\mu) \frac{n-1}{(2n-3)^{1/2}} + p_n(\mu) \frac{n}{(2n+1)^{1/2}} \right) \right], \quad (\text{A.8}) \end{aligned}$$

which allows the μ^2 term to be removed from the integral.

The expansion is truncated to order N and to determine the eigenstructure the following equation needs to be solved:

$$\mathbf{A} \mathbf{r}_n = \lambda_n \mathbf{r}_n, \quad (\text{A.9})$$

where $\mathbf{r}_n$ is an eigenvector and λ_n is an eigenvalue.

Evaluating this expression explicitly yields:

$$\begin{pmatrix} \frac{1}{3} & \frac{2}{3\sqrt{5}} & 0 & 0 \\ \frac{2}{3\sqrt{5}} & \frac{3^2}{35} + \frac{2^2}{15} & \frac{4}{7\sqrt{5}} & 0 \\ 0 & \frac{4}{7\sqrt{5}} & \frac{5^2}{99} + \frac{4^2}{63} & \ddots \\ 0 & 0 & \ddots & \ddots \end{pmatrix} \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} \frac{1}{3}r_1 + \frac{2}{3\sqrt{5}}r_2 \\ \frac{2}{3\sqrt{5}}r_1 + \left(\frac{3^2}{35} + \frac{2^2}{15}\right)r_2 + \frac{4}{7\sqrt{5}}r_3 \\ \frac{4}{7\sqrt{5}}r_2 + \left(\frac{5^2}{99} + \frac{4^2}{63}\right)r_3 \\ \vdots \end{pmatrix} = \lambda_n \begin{pmatrix} r_1 \\ r_2 \\ r_3 \\ \vdots \end{pmatrix}. \quad (\text{A.10})$$

The rows of this expression appear to resemble the recurrence relationship in eq. (A.8) if the r_n are Legendre polynomials. In order for this, the eigenvalue problem, to hold the r_n must be the Legendre polynomials evaluated at μ_n

$$\mathbf{r}_n = (p_0(\mu_n), p_2(\mu_n), \dots, p_{N-1}(\mu_n))^T, \quad (\text{A.11})$$

where

$$\mu_n \in \{\mu_n : p_{N+1}(\mu_n) = 0\}. \quad (\text{A.12})$$

The eigenvalues are then given by:

$$\lambda_n = \mu_n^2. \quad (\text{A.13})$$

Appendix B

Effective Diffusion Coefficients for the Semi-Analytic Nodal Method

In the Semi-Analytic Nodal Method (SANM) the group fluxes are expanded as

$$\phi(u) = \mathbf{a}_0 + u\mathbf{a}_1 + \left(u^2 - \frac{h^2}{3}\right)\mathbf{a}_2 + \left(\sinh \sqrt{\hat{\mathbf{S}}}u\right)\mathbf{a}_3 + \left(\cosh \sqrt{\hat{\mathbf{S}}}u\right)\mathbf{a}_4, \quad (\text{B.1})$$

where $\hat{\mathbf{S}}$ is a diagonal matrix and the $\mathbf{a}_m$'s are vectors of expansion coefficients. Considering only one group the surface fluxes and currents are given by

$$\phi_{\pm} = \pm ha_1 \pm \left(\sinh h\sqrt{\hat{S}}\right)a_3 + e_{\phi}, \quad (\text{B.2})$$

$$J_{\pm} = -D \left[a_1 + \left(\sqrt{\hat{S}} \cosh h\sqrt{\hat{S}}\right)a_3 \right] \pm e_J, \quad (\text{B.3})$$

where

$$e_\phi = a_0 + \frac{2}{3}h^2a_2 + \left(\cosh h\sqrt{\hat{S}}\right)a_4, \quad (\text{B.4})$$

$$e_J = -D \left[2ha_2 + \left(\sqrt{\hat{S}} \sinh h\sqrt{\hat{S}}\right)a_4 \right]. \quad (\text{B.5})$$

Defining

$$C_j = \frac{\tanh \sqrt{\hat{S}}h}{\sqrt{\hat{S}}h}, \quad (\text{B.6})$$

and rearranging eq. (B.3) gives

$$\frac{\sinh \sqrt{\hat{S}}h}{h}a_3 = -\frac{C_j J_\pm}{D} - C_j a_1 \pm \frac{C_j}{D}e_j. \quad (\text{B.7})$$

Substitution into eq. (B.2) and subsequent simplification yields

$$\phi_\pm = \pm ha_1 \mp h \left(C_j \frac{J_\pm}{D} + C_j a_1 \right) - C_j 2h^2 a_2 + a_0 + \frac{2}{3}h^2 a_2 + \frac{a_4}{\cosh \sqrt{\hat{S}}h}. \quad (\text{B.8})$$

Preservation of the node average flux can be expressed as

$$a_0 + B_0 a_4 = \bar{\phi}, \quad (\text{B.9})$$

where

$$B_0 = \frac{\sinh \sqrt{\hat{S}}h}{\sqrt{\hat{S}}h}. \quad (\text{B.10})$$

Using the expression above to simplify eq. (B.8) results in

$$\phi_{\pm} = \mp h C_j \frac{J_{\pm}}{D} + C_f \bar{\phi} + (1 - C_f) a_0 \pm h(1 - C_j) a_1 + 2h^2 \left(\frac{1}{3} - C_j\right) a_2, \quad (\text{B.11})$$

where

$$C_f = \frac{2\sqrt{\hat{S}}h}{\sinh 2\sqrt{\hat{S}}h}. \quad (\text{B.12})$$

This can be written more concisely as

$$\phi_{\pm} = \mp h C_j \frac{J_{\pm}}{D} + C_f \bar{\phi} + T_{\pm}, \quad (\text{B.13})$$

where the definition of $T_{\pm}$ is implied.

The similarity of eq. (B.13) to those given in the derivation of the Effective Diffusion Coefficient (EDC)s^{64,65} should be clear at this stage. The next step is to use the expression derived above and apply it to the two-node problem to obtain the EDCs.

To differentiate between the two nodes the superscripts L and R are used for the left and right node at a given interface. Enforcing the continuity of the surface flux at the boundary results in

$$-h^L C_j^L \frac{J_+^L}{D^L} + C_f^L \bar{\phi}^L + T_+^L = h^R C_j^R \frac{J_-^R}{D^R} + C_f^R \bar{\phi}^R + T_-^R. \quad (\text{B.14})$$

Realising that $J_+^L = J_-^R = J$ allows us to write

$$J = -(\bar{D}^R \bar{\phi}^R - \bar{D}^L \bar{\phi}^L) \quad (\text{B.15})$$

where

$$\overline{D}^R = \left[\frac{h^L C_j^L}{D^L} + \frac{h^R C_j^R}{D^R} \right]^{-1} \left(C_f^R + \frac{T_-^R}{\phi^R} \right) \quad (\text{B.16})$$

$$\overline{D}^L = \left[\frac{h^L C_j^L}{D^L} + \frac{h^R C_j^R}{D^R} \right]^{-1} \left(C_f^L + \frac{T_+^L}{\phi^L} \right) \quad (\text{B.17})$$

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