

SOLUTION OF THE MULTIGROUP ANALYTIC NODAL DIFFUSION EQUATIONS IN 3-DIMENSIONAL CYLINDRICAL GEOMETRY

RIAN H. PRINSLOO

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Supervisor: Prof. H. Moraal
Co-supervisor: Dr. D.I. Tomašević

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Abstract

Nodal diffusion methods have been used extensively in nuclear reactor calculations, specifically for their performance advantage, but also their superior accuracy. In this work a nodal diffusion method is developed for three-dimensional cylindrical geometry. Recent developments in the Pebble Bed Modular Reactor (PBMR) project have sparked renewed interest in the application of different modeling methods to its design, and naturally included in this effort is a nodal method for cylindrical geometry. More specifically, the Analytic Nodale Method (ANM) has been applied to numerous reactor problems with much success. The multi-group ANM is applied to Cartesian geometry in the Necsa developed OSCAR-3 code system used for the calculation of MTR and PWR type nuclear reactors. However, in support of the PBMR project, a need has arisen to include the ANM in cylindrical geometry.

The ANM is based on a transverse integration principle, resulting in a set of one-dimensional equations containing inhomogeneous sources. The issue of applying this method to 3D cylindrical geometry has never been satisfactorily addressed, due to difficulties in performing the transverse integration, and a proposed solution entails the use of conformal mapping in order to circumvent these difficulties. This approach should yield a set of 1D equations with an extra, geometrically dependent, "ghost" source. This thesis describes the mathematical development of the conformal mapping approach, as well as the numerical analysis via a developed FORTRAN test code. The code is applied to a series of test problems, ranging from idealized constructions to realistic PBMR 400 MW designs. Results show that the method is viable and yields much improved accuracy and performance, similar to what may be expected from nodal methods.

Samevatting

Nodale diffusiemetodes word ekstensief gebruik in kernreaktorberekeninge, spesifiek vir die spoed- en akkuraatheidsvoordele wat hulle bied. In hierdie verhandeling word 'n nodale diffusiemetode ontwikkel vir die gebruik in meer-groep, drie-dimensionele silindriese geometrie. Die onlangse verwikkelinge rakende die Korrelbedreaktorprojek het 'n nuwe inspuiting aan berekeningsmetodes vir sulke reaktore gegee en die silindriese nodale diffusiemetode is 'n belangrike bousteen van so 'n berekeningstelsel. Die Analitiese Nodale Metode (ANM) word met groot sukses in hierdie veld van globale reaktorberekeninge gebruik. Hierdie metode is ten volle geïmplementeer in Kartesiese geometrie in die Necs-a-ontwikkelde OSCAR berekeningstelsel. Met die oog op die ondersteuning van die Korrelbedreaktorprojek, het die behoefte ontstaan om 'n silindriese oplossingsmetode by hierdie sisteem te voeg.

Die ANM word baseer op die beginsel van transversale integrasie, wat 'n reeks een-dimensionele vergelykings tot gevolg het. Elk van hierdie vergelykings bevat 'n stel nie-homogene bronne en kan analities opgelos word. Die toepassing van hierdie metodiek op silindriese geometrie is nog nie in die verlede suksesvol aangespreek nie, aangesien daar wiskundige struikelblokke in die transverse integrasie proses is. In hierdie verhandeling word 'n moontlike oplossing, via die gebruik van die konforme afbeeldingstechniek, bespreek. Hierdie metode behoort ook 'n stel een-dimensionele vergelykings te produseer, maar in hierdie geval met 'n ekstra, nie-homogene, geometries-afhanklike bron. Die wiskundige ontwikkeling en numeriese evaluasie van hierdie metode (via 'n ontwikkelde FORTRAN toetskode) word in hierdie werk beskryf, en resultate word verskaf vir beide geïdealiseerde opstellings en realistiese korrelbedprobleme. Resultate dui daarop dat die metode aan die tipiese standaarde van nodale metodes voldoen.

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Contents

1	INTRODUCTION	9
1.1	Reactor calculational methods and the South African nuclear industry	9
1.2	Core solution methods in cylindrical geometry	10
1.3	PBMR background	12
1.4	Nodal methods	15
1.5	Goals of this thesis	18
1.6	Layout of the thesis	19
2	DEVELOPMENT OF A 3D FINITE-DIFFERENCE SOLVER	21
2.1	Introduction	21
2.2	Geometric description	22
2.3	Finite-difference equations in 3D cylindrical coordinates	24
2.4	3D solution process - the 7-point equations	28
2.4.1	Numerical implementation of solution	33
2.5	Code implementation and testing	35
2.6	Conclusion	41
3	DERIVATION OF ANALYTIC NODAL METHOD IN CYLINDRICAL GEOMETRY	42
3.1	Introduction	42
3.2	Balance equation in three dimensions	43
3.3	Conformal mapping	46
3.3.1	Relationship between mapped and unmapped quantities	50
3.4	Transverse integration of mapped equations	53
3.4.1	Transverse integration over v : the u -equation	53
3.4.2	Transverse integration over u : the v -equation	55
3.4.3	Transverse integration over (r, θ) - the z -equation	61
3.4.4	Summary	63

3.5	Solution to the one-dimensional v -equation	63
3.5.1	Calculation of moments	67
3.5.2	Current and flux expressions	70
3.5.3	Tensorial source	72
3.6	Solution to the one-dimensional v -equation	76
3.6.1	Determination of source moments	78
3.6.2	Current and flux expressions	81
3.6.3	Tensorial source	82
3.7	Solution to the one-dimensional z -equation	84
3.7.1	Determination of source moments	86
3.7.2	Current and flux expressions	87
3.7.3	Tensorial source	88
3.8	Balance equation	88
3.9	Transverse leakage approximation	89
3.10	Conclusion	94
4	FINE-MESH LIMIT	96
4.1	Introduction	96
4.2	Axial direction	98
4.3	Radial direction	100
4.4	Azimuthal direction	102
4.5	Fine-mesh expressions in the center	104
4.6	Conclusion	106
5	NODAL CODE VALIDITY	108
5.1	Introduction	108
5.2	Test code description	109
5.3	Hollow cylinder problem	110
5.4	“Striped” (r, θ) problem	114
6	RESULTS AND DISCUSSION	120
6.1	Dodds’ benchmark application	120
6.2	PBMR application	122
6.3	IAEA cylindrical 3D benchmark	131
7	CONCLUSIONS AND FUTURE WORK	143
7.1	Introduction	143

7.2	General conclusions	144
7.3	Future work	146
7.4	Final considerations	146
A	TEST CODE USER MANUAL	148
B	DODDS BENCHMARK PROBLEM	161
C	TEST CODE INPUT EXAMPLES	163
D	IAEA BENCHMARK DESCRIPTION (CYLINDRICAL)	168
E	RECURRENCE RELATIONSHIPS FOR FLUX MOMENTS	173
E.1	Flux moments	173
E.2	Mapped flux moments	175
F	EXPANSIONS FOR DOUBLE LEGENDRE INTEGRALS	177
G	TRANSVERSE LEAKAGE QUADRATIC FIT	181

List of Figures

1.1	3D cylindrical discretization scheme	11
1.2	PBMR 400 MW schematic core layout	14
1.3	PBMR fuel design	15
2.1	Azmi's (r, z) fixed source benchmark problem illustration	37
2.2	DODDS' benchmark model in (r, z) geometry	39
3.1	Conformal mapping - cylindrical to rectangular mapping	48
5.1	Infinite cylinder flux and eigenvalue error trends - 2nd order expansion	113
5.2	(r, θ) "Striped" problem geometric description	115
5.3	Reference solution for the "Striped" problem	116
5.4	"Striped" problem flux error (radial profile) along source zone	118
5.5	"Striped" problem flux error (radial profile) along absorber zone	118
6.1	Dodds 2D (r, z) - radial profile (axially-averaged)	121
6.2	Dodds 2D (r, z) - axial profile (radially-averaged)	122
6.3	PBMR 2D (r, z) material layout	123
6.4	3D PBMR 400 - (r, θ) projection (not to scale)	125
6.5	FD convergence error vs performance (calculational time)	126
6.6	PBMR benchmark radial multi-group flux profiles (axially-averaged)	127
6.7	PBMR benchmark axial multi-group flux profiles (radially-averaged)	128
6.8	3D FD convergence error vs performance (calculational time)	129
6.9	PBMR: Radial profile through and adjacent to control	130
6.10	PBMR: Group fluxes through control - azimuthal profile	131
6.11	IAEA (r, z) layout - azimuthal cut at 45 degrees	132
6.12	IAEA (r, z) layout - azimuthal cut at 0 degrees	133
6.13	IAEA (r, θ) layout - top view	133
6.14	IAEA eigenvalue extrapolation - 2nd order fit for uniform refinement	135
6.15	IAEA (r, z) thermal flux errors - (a) quadratic leakage (b) flat leakage	136

6.16	IAEA (r, θ) thermal flux errors - (a) quadratic leakage (b) flat leakage	137
6.17	IAEA thermal profiles	138
6.18	IAEA radial thermal profile through axial top of core	138
6.19	IAEA thermal flux errors for the mixed leakage approximation	140
6.20	IAEA nodal aspect ratios	141
B.1	DODDS' benchmark model in (r, z) geometry	161
D.1	IAEA (r, z) layout - azimuthal cut at 45 degrees	168
D.2	IAEA (r, z) layout - azimuthal cut at 0 degrees	169
D.3	IAEA (r, θ) layout - top view	169
D.4	IAEA Nodal mesh - bottom reflector and bottom core regions	170
D.5	IAEA Nodal mesh - top core and top reflector regions	171

List of Tables

2.1	Description and result of an infinite homogeneous cylinder	36
2.2	Azmi's fixed source (r, z) verification problem	38
2.3	DODDS' benchmark description and results	40
5.1	Nodal results for hollow cylinder problem	112
5.2	"Striped" problem global results	117
6.1	Eigenvalue results for 2D Dodds' benchmark problem	120
6.2	2D PBMR global results (nodal vs FD)	126
6.3	3D PBMR global results (nodal vs FD)	129
6.4	Eigenvalue results for 3D IAEA benchmark problem	134
6.5	Eigenvalue results for IAEA benchmark - mixed leakage approximation	140
B.1	DODDS' benchmark cross-section description	162
D.1	IAEA Material cross-sections	171

Chapter 1

INTRODUCTION

1.1 Reactor calculational methods and the South African nuclear industry

The nuclear industry is carefully emerging from an era it would best forget. For many years, partly due to international politics and partly due to accidents such as Chernobyl and Three Mile Island, the nuclear landscape was bleak and empty, with very few countries actively developing new technologies, and building new reactors. In the more recent past, the momentum has built up once again in this industry, and pockets of new and existing technology development have opened up in various countries.

South Africa has played an active part in this resurgence, largely in the form of the Pebble Bed Modular Reactor (PBMR) initiative - a generation IV reactor concept based upon older German technology. It would be a blatant understatement to say that the design and creation of a nuclear power plant is a complex process, and many specialized disciplines have to merge and overlap synergistically in a field with carefully controlled margins. At the heart of such development surely would lie the design of the nuclear reactor core, and would entail specialist areas such as neutronic design, thermal hydraulic design, reactor kinetics and system dynamics.

Within these fields the primary focus is on safety, and to this end computer simulations have become an invaluable tool. The ability to predict accurately quantities such as neutron and temperature distribution during operating, as well as accident conditions, dose levels during maintenance, and operational parameters such as criticality, cycle length and power levels are central to the design and operation of nuclear reactors.

This thesis falls within the domain of neutronic analysis and presents a method for determining the flux distribution throughout the reactor core in an accurate and efficient

manner. Typically, such a flux distribution is obtained in two phases:

1. Detailed neutron transport calculations in fine energy groups to produce accurate flux- and volume weighted cross-sections for each material region in the core. This calculation is independently performed for each material region, and cross-sections are typically tabulated against relevant state parameters. This is a once-off process and results in a library of average cross-sections in broad energy groups and large homogenized material regions.
2. The average cross-sections obtained in the previous step are used as input data for global core diffusion calculations. These calculations result in core wide-flux and power profiles. Diffusion methods are derived as an approximation to neutron transport and are therefore less accurate, but provide a substantial performance increase. Nevertheless, these calculations are run very often, both within the realm of steady-state and time-dependent solutions, and require even further performance improvements. This point approaches the subject of this thesis, and to be more specific, as it is applied to cylindrical reactor core designs.

This two step process is described in more detail in [3].

1.2 Core solution methods in cylindrical geometry

In this work we will restrict ourselves to full core calculational flux solutions for which region-homogenized cross-sections have been appropriately prepared. If we further assume that such systems are adequately described by the neutron diffusion equation, (which qualitatively assumes that the angular neutron flux is linearly anisotropic), we may proceed to describe the flux distribution within an annular cylindrical reactor by writing the three-dimensional diffusion equation in cylindrical geometry. We present the steady-state form of this equation here purely for illustration, and will attack it in a more rigid mathematical sense much later.

$$-\nabla \cdot [D^g(r, z, \theta) \nabla \Phi^g(r, z, \theta)] + \sigma^{g,rem}(r, z, \theta) \Phi^g(r, z, \theta) - Q^g(r, z, \theta) = 0 \quad (1.1)$$

Here $D^g(r, z, \theta)$ denotes the diffusion coefficient, and $\sigma^{g,rem}(r, z, \theta)$ the effective removal cross-section. In eq. (1.1) $Q^g(r, z, \theta)$ represents both the fission and scattering. Eq. (1.1) is the problem we will later need to solve in order to obtain the criticality level of the core, as well as the position and energy dependent distribution of the flux. We may attempt to rewrite this equation in a more quantitative and understandable manner, by reshaping it as an equation for average fluxes and currents. If we divide the system into n zones (nodes),

as in Figure 1.1 below, integrate the diffusion equation over each zone and then divide the equation by node volume, we will obtain a set of coupled 3D balance equations over all nodes n . The details of this process will be described later and are not important here. What is of importance, is that we have divided the heterogeneous system into a discretized set of homogeneous zones, or nodes.

$$\sum_{j=1}^6 a_n^{r,j} \bar{J}_{jn} + \sigma_n^{rem} \bar{\Phi}_n \approx Q_n \quad (1.2)$$

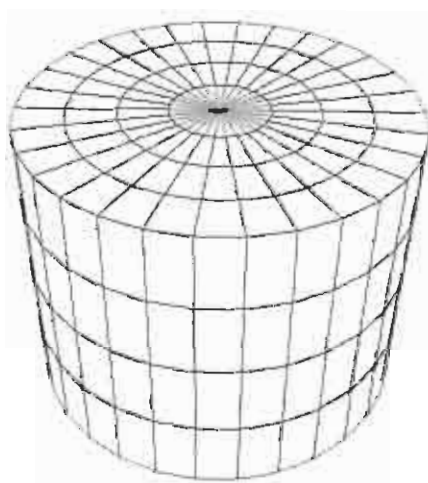


Figure 1.1: 3D cylindrical discretization scheme

In eq. (1.2) $\bar{\Phi}_n$ represents the node-averaged flux and $\bar{J}_{jn}$ the side averaged net current from node n to neighbour j . The surface-to-volume ratio for each bounding surface is denoted by $a_n^{r,j}$. This representation of the diffusion problem is much more intuitive, and allows one to view the nodal equation as a balance of currents leaking out of all six sides of the node (term 1), removals from the node and energy group (term 2), and sources adding neutrons to the node and energy group in the form of fission or in-scattering (right hand side term). In writing eq. (1.1) in this form, we have also accepted that we are only interested in average quantities for each node, and since this is the case, eq. (1.2) also takes the form of the equation we attempt to solve in this thesis. Before we can solve eq. (1.2), which is one equation with multiple unknowns, we need a further relationship between node-averaged flux and side-averaged currents in each direction. In attempting to find such a relationship,

suitable to the given problem and, as importantly, find it in an effective and efficient manner, we require some special considerations.

The performance of any given discretized solution is defined by both the number of nodes in the system, and the cost of each intra-node calculation. The individual node volumes, and therefore number of nodes in the system, are influenced by the following factors:

1. Regions of constant homogenized cross-section. This consideration is complex in nature, but in the case of light water reactor calculations, is typically chosen to be in the order of a fuel assembly. Within e.g. the PBMR reactor, this concept is not a priori defined because of the absence of fixed fuel assemblies with well-defined dimensions. This consideration typically sets the maximum diffusion node size.
2. Material interfaces, which influence the magnitude of flux gradients within the reactor.
3. Accuracy of solution method: The greater the analytic accuracy of each intra-node solution, the larger the node size can be in order to recover the detailed reference solution within the node. If therefore, with this in mind, we obtain the missing relationship in eq. (1.2) via a finite-difference (FD) approximation (described in Chapter 2), the node size is typically limited to the order of a diffusion length in each part of the system. In the case of nodal methods, and specifically the ANM, the relationship used involves an analytic solution of the intra-node flux (described in Chapter 3), and hence can accommodate much larger nodes (5-8 diffusion lengths). This constitutes an important potential for performance increase.

These considerations are at play when the required efficiency (referring to the combination of accuracy and performance) of a solution algorithm is to be determined. If we return to the issue of solving eq. (1.2), these factors are to be carefully considered when choosing a solution method, and in this case, in defining the node-averaged flux to side-averaged current relationship. Nevertheless, whatever the outcome may be, it is clear from the above considerations that nodal methods potentially provide an important performance improvement and in Section 1.4 we will present a brief discussion of nodal methods in general, and the Analytic Nodal Method (ANM) in particular. However, we first give a short description of the South African PBMR, the industrial application area of the work in this thesis.

1.3 PBMR background

The application of this thesis does not lie solely with the PBMR, but with any reactor definable by areas of constant, cylindrically discretized, homogenized regions. Nevertheless,

the current South African PBMR project signifies a direct application for this work and therefore deserves some attention. The following extract regarding its background is taken from [18].

“Gas-cooled reactors have had a long and varied history dating back to the very early days of the development of nuclear energy. The development proceeded along an evolutionary path together with significant advances in supporting technologies, and in South Africa has culminated in the design of the Pebble Bed Modular Reactor (PBMR). The PBMR is expected to achieve the goals of safe, efficient, environmentally acceptable and economic production of energy at high temperature for the generation of electricity and industrial process heat applications. The PBMR power conversion is based on a single loop direct Brayton thermodynamic cycle, with a helium-cooled and graphite-moderated nuclear core assembly as heat source. The coolant gas transfers heat from the core directly to the power conversion system, consisting of gas turbo-machinery, a generator, gas coolers and heat exchangers.”

The design of the reactor core is given briefly in Figure 1.2, and highlights some of the major features important to the safety and efficiency of the design.

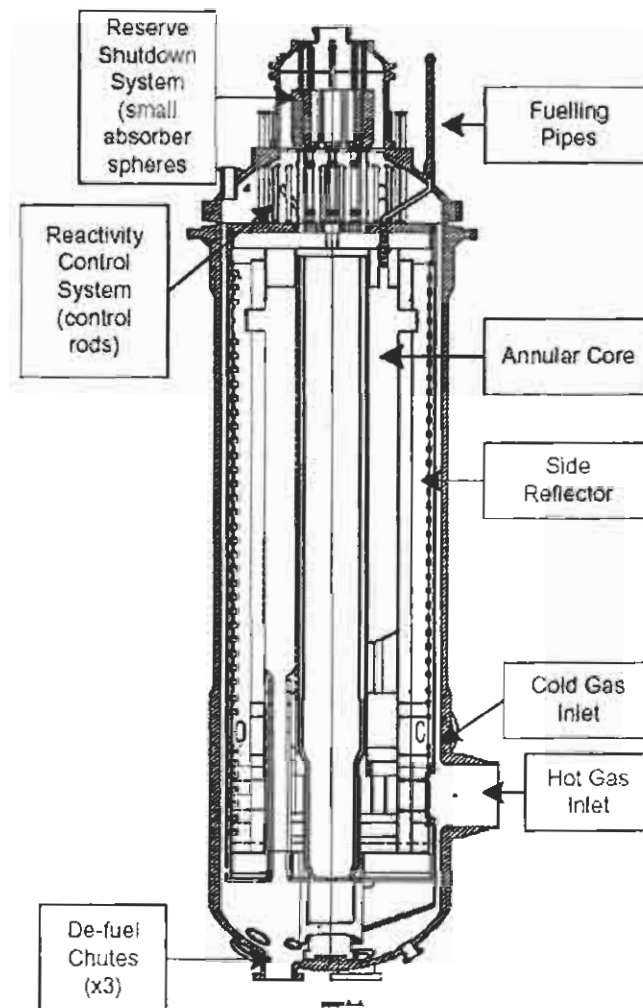


Figure 1.2: PBMR 400 MW schematic core layout

The reactor exhibits some interesting characteristics, such as on-line fuel loading (minimizing excess reactivity), a fixed inner reflector, and control rods placed within borings in the side reflector. Fuel elements are in the form of graphite fuel spheres or pebbles, containing fine kernels of low enriched Uranium. At any given time the core will be filled by approximately 400 000 fuel spheres, each containing about 15 000 fuel kernels. The fuel design is shown in Figure 1.3.

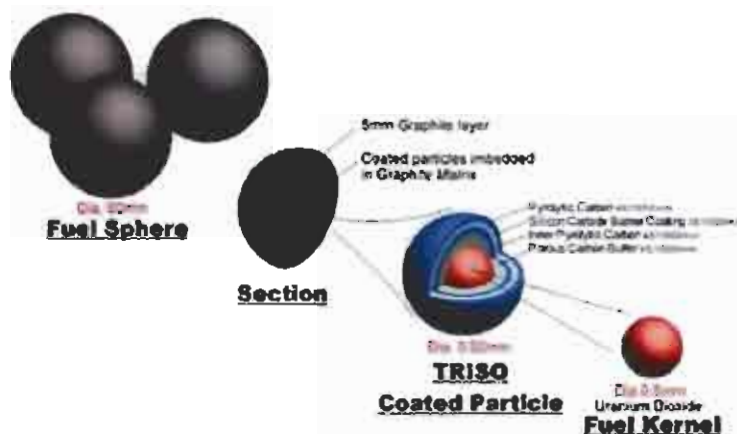


Figure 1.3: PBMR fuel design

It is clear that the typical calculational approach of choosing fuel assemblies (in this case individual pebbles) as homogenization zones would not be feasible, and therefore PBMR calculations are performed on homogenization zones defined by other factors such as regional burnup, changes in flux spectra, and drastic changes in material parameters. These issues, although not the topic of this thesis, play an important role regarding the calculational efficiency, as referred to by the arguments in Section 1.2.

1.4 Nodal methods

General characteristics

The class of nodal methods, as applied to full reactor core diffusion problems, has grown into a mature and trusted technique in recent times. Nodal formalisms have gained much favour due to their increased performance and accuracy, and mostly share three characteristics [13].

1. Unknowns are defined in terms of volume-averaged fluxes and surface-averaged net or partial currents.
2. The volume (node) averaged fluxes and surface-averaged currents are related through auxiliary relationships. Such relationships, in the case of modern nodal methods, are often obtained via a transverse integration procedure. In older classes of nodal methods, termed nodal simulators, these relationships were typically obtained via auxiliary fine-mesh finite-difference calculations.

3. Transverse leakage terms appear due to the transverse integration procedure, and these are approximated in some way. Typical approaches would include the “flat leakage” approximation, and the “quadratic leakage” approximation. The latter introduces a three node quadratic fit for the transverse leakage term in the transversely integrated equations and has become the industry standard in Cartesian geometry.

Beyond these similarities, methods differ largely in the form of the intra-node solution. Two classes of methods, which are most often utilized, are the analytic nodal method (ANM), and the polynomial method. In the case of the analytic method, the intra-node flux shape is solved directly from the one-dimensional transversely integrated diffusion equations in each direction. This approach requires no approximations other than the transverse leakage approximation in point three above. In one dimension, therefore, the analytic method is exact. A full description concerning the Analytic Nodal Method may be found in [11] and Chapter 3 contains a detailed description of this approach.

In the case of the polynomial methods, the intra-node one-dimensional flux is approximated as an n^{th} order polynomial on some set of basis functions. Expansion coefficients may be determined in various ways, and the transverse leakage approximation is, of course, still required. It may be noted that, in the case of these polynomial methods, the one-dimensional flux, and therefore both the scattering and fission sources in the one-dimensional equations, are approximated. Further details concerning the polynomial method may be found in [15].

The pros and cons of these methods do not lead to any clear preference in selection, but some arguments [13] suggest that the ANM does exhibit both slight performance and accuracy advantages over its polynomial counterpart. Other classes of nodal methods, which do not require transverse integration, also exist and may be solved via various approaches such as direct polynomial expansion, analytic solution, response matrix formalism and plane wave approximation.

Cylindrical geometry

In this development, the focus will be placed upon the Analytic Nodal Method. The ANM in Cartesian geometry has been implemented and used within the Necsa developed OSCAR code system for some years, and extended to a full multi-group ANM formalism [14]. Given the views in Section 1.1, the need has been identified to extend the OSCAR system to include the ANM in cylindrical geometry, for possible application within the arena of PBMR design, safety and core-follow calculations. It is important to examine the landscape of nodal methods in cylindrical geometry prior to such a development effort, and be aware of the potential pitfalls and successes within this domain.

1. The ANM is based on a transverse integration principle, resulting in a set of one-dimensional equations containing inhomogeneous sources. The issue of applying this method to 3D cylindrical geometry has never been satisfactorily addressed. Ougouag [12] showed that the traditional transverse integration fails in producing a one-dimensional equation in the θ -direction. Instead, he proposed a two-dimensional solution in r and θ . This yields a set of equations that is analytically rather complex and difficult to implement practically, and that is, at the time of this writing, still under development.
2. The polynomial class of methods has been applied to 3D cylindrical geometry, an example of which may be found in the NEM (Nodal Expansion Method) code system. Very limited 3D results are available.
3. Within the class of analytic function expansion methods, Cho [19] suggests a solution utilizing a set of analytic base functions for a direct 3D solution. This approach shows some promise, but some closer efficiency evaluation is necessary due to the large number of unknowns per node.
4. Implementation of a nodal integral method for 2D (r, z) geometry has been developed [6].
5. Within the PBMR project, so called core-follow calculations are currently performed with the CITATION [9] code (or adaptation thereof), utilizing a finite-difference solution method.
6. In the implementation of the ANM in hexagonal geometry, which also suffers from analytic difficulties, an approach was suggested by Chao [16] which entails the use of conformal mapping to simplify the geometry of the problem.

From the above perspectives, the development of the ANM in 3D cylindrical geometry is an outstanding issue, specifically within the context of the South African nuclear industry and the PBMR project. In this work, the development of the ANM in cylindrical geometry is undertaken, utilizing the technique of conformal mapping to circumvent the transverse integration difficulties experienced in a straight-forward application of the ANM. This approach could potentially circumvent the issue in (1) above.

1.5 Goals of this thesis

Some background surrounding the area of concern has been sketched, and a more concise formulation of the problem is now possible. The aim of this work, therefore, may be stated as a need to draw relevant conclusions regarding two main issues:

1. Does the proposed conformal mapping technique allow, for the first time, the formulation and implementation of an Analytic Nodal Method in cylindrical geometry? The assumptions within the nodal formalism, and furthermore within the conformal mapping approach (as suggested in this work), are difficult to quantify analytically, and some aspects of these conclusions will have to be drawn from numerical arguments. The method will have to adhere to the levels of performance and accuracy expected from the ANM.
2. Is the proposed solution applicable to the PBMR design, and can such a development add value to the reactor calculations within the PBMR project? This question is not directly analogous to point (1) above, due to the consideration mentioned in Section 1.2. The PBMR reactor design is sufficiently different from typical light water reactors (LWR) to invalidate, or substantially influence, much of the experience gained from applying nodal methods to LWRs.

In the course of addressing these issues, a series of papers has been produced, each signifying an important milestone within the work. These papers are listed and described below.

1. Rian H. Prinsloo, Djordje I. Tomašević, "Development of the Analytic Nodal Method in Cylindrical Geometry," *Proceedings of Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Application 2005*, Avignon, France, September 2005 on CD (2005). This publication describes the mathematical method development, and illustrates its basic viability via simplified idealized numerical examples. The paper received an invitation for publication in the *Journal for Nuclear Science and Engineering* (NSE).
2. Rian H. Prinsloo, et al., "Application of SP2 and the Spatially Continuous SP2-P1 Equations to the PBMR Reactor," *Proceedings of Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Application 2005*, Avignon, France, September 2005 on CD (2005). In the course of this work, some interesting fringe topics of potential future importance to PBMR modeling methods were explored. This paper signifies one such investigation, but one which falls somewhat outside the scope of this thesis.

3. Rian H. Prinsloo, Djordje I. Tomašević, "Development of the Analytic Nodal Method in Cylindrical Geometry for PBMR Application", 3rd International Topical Meeting on High Temperature Reactor Technology (HTR 2006), Johannesburg, South Africa, October 2006 on CD (2006). This paper addresses the major goals of this thesis, and applies the completed nodal methodology to the PBMR reactor design. The paper received both an award for best research paper by a young researcher as well as an invitation for publication in the Journal for Nuclear Engineering and Design (NED). The NED paper will be submitted early in 2007.
4. Rian H. Prinsloo, Djordje I. Tomašević, "Approach to Singular Regions in the Conformally Mapped Analytic Nodal Method in Cylindrical Geometry", Submitted and accepted for publication at Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Application 2007, Monterey, California, USA, April 2007 (2007).

1.6 Layout of the thesis

The thesis layout will follow, in most respects, the order in which the development of this project was performed. Chapter 2 will trace the development of a finite-difference based test code, which is used to produce reference results for the proposed ANM based test code to come. This development will be similar in nature to the code system currently used by PBMR for full-core solutions (see 1.4 above). Hereafter, the development and mathematical basis for the cylindrical ANM is described in Chapter 3. This chapter forms the heart of the thesis, since the mathematical formulation represents the major contribution in this work. Apart from the use of conformal mapping, other relevant issues such as the nature of the transverse leakage approximation in cylindrical geometry, are formulated here. Chapter 4 addresses the existence of a fine-mesh limit for the developed conformal mapping approach. This issue is important for numerical stability and accuracy of the method.

Chapters 5 and 6 numerically apply the nodal approach to idealized and realistic problems respectively, and show the advantages, pitfalls, and potential improvements associated with the proposed approach. Chapter 5 investigates the domain of applicability of the nodal method, and addresses issues such as the treatment of severe azimuthal inhomogeneity, as well as the effect of the center cut-out approximation required by conformal mapping. Specifically, the application of the method to the PBMR 400 MW benchmark problem in Chapter 6, gives some insight into the relevance of the method for its intended area of application. Conclusions and future work are described in Chapter 7.

The reader is reminded that the work is eventually intended for application within an already developed industrial code system [22], and will be placed within the appropriate infrastructure upon successful proof of concept demonstration, in which this thesis plays an important part.

A foundation has now been laid, on top of which the technical description will be built, and the process starts in the next chapter with the development and verification of the finite-difference test code, **SciFi**, which will be used to validate the proposed nodal method. The name refers to the obvious application of the code, namely **SC**ilindrical **FI**nite difference, but hopefully also conveys the underlying attraction within any and all scientific development: The vision to transform **SC**ience **FI**ction into science fact...

Chapter 2

DEVELOPMENT OF A 3D FINITE-DIFFERENCE SOLVER

2.1 Introduction

Before proceeding with the development of a nodal method, we must address the question of a reference or benchmark against which the success or failure of the nodal method may be measured. Such a measure will be with respect to both accuracy and speed. One option may entail utilizing an off-the-shelf cylindrical finite-difference calculational code, and one may mention the CITATION [9] finite-difference code as an example, which is currently used by PBMR and was noted in Section 1.4. This finite-difference solution scheme utilized by PBMR results in very long calculational times, and in some cases reduced accuracy in order to make such calculations practical.

The approach to use such an existing code, like CITATION, as reference for the nodal methodology to come, could accelerate the initial development of this work, but a price may be paid in the latter stages due to a lack of flexibility. For this reason, the decision was made to begin the work with the development and implementation of a custom 3D cylindrical finite-difference solver. Such a development has the following advantages:

- Opportunity to customize the functionality according to project requirements, and to allow updates during the project development.
- Establishment of both a mathematical and a coding skeleton for the nodal development, since many concepts are analogous within the finite-difference and nodal formalisms.
- Introduction of mathematical notation within a less complex environment.

- The potential to obtain relevant timing comparisons between nodal and finite-difference codes, since similar acceleration schemes will be built into both codes.

The current chapter, therefore, is concerned with deriving and implementing the finite-difference approximation [1], as applied to the multi-group neutron diffusion equation in cylindrical coordinates. The derivation is carried out in three dimensional (r, z, θ) geometry and will culminate in the development of a FORTRAN based numerical code. The chapter will follow the approach of solving the within-group problem (diffusion equation for a single energy group). In such an approach each within-group diffusion equation would contain a generic multi-group source term, built up from a combination of a fixed, a scattering and a fission source (as the problem requires). These sources (non-linear in the case of multi-group scattering and fission sources) may be resolved via an iterative process. The domain is assumed to be discretizable into cylindrical segments, with material parameters constant and appropriately averaged within each zone.

The derivation presented in the remainder of this chapter does not constitute new work, and finite-difference-based solutions for the neutron diffusion equation in three dimensional cylindrical geometry represent a standard (although inefficient) approach. Some alternatives within such a formalism may be found in [2], including the mesh centered scheme chosen within this chapter. Nevertheless, the finite-difference equations are developed in this chapter in some detail due to the reasons just presented.

2.2 Geometric description

Before we construct the finite-difference equations required to implement a reference cylindrical solver, we introduce the following notation in order to discretize the domain in r, z and θ coordinate directions:

- $r = r_0, r_1, \dots, r_N$ describes the radial mesh boundaries, with r_0 at the center - enumerated by index $s : 0, 1, 2 \dots N$.
- Further define the radial mesh width $\Delta r_s = r_{s+1} - r_s$.
- $\theta = \theta_0, \theta_1, \dots, \theta_P$ describes the azimuthal mesh boundaries, with θ_0 as the 0 degree angle (counter-clockwise rotation) - enumerate by index $u : 0, 1, 2 \dots P$ with $\theta_0 = \theta_P$.
- Further define the azimuthal mesh width as $\Delta \theta_u = \theta_{u+1} - \theta_u$.
- $z = z_0, z_1, \dots, z_M$ describes the radial mesh boundaries, with z_0 at the bottom - enumerated by index $t : 0, 1, 2 \dots M$.

- Further define the axial mesh width $\Delta z_t = z_{t+1} - z_t$.

The following notational constructs are adopted for the remainder of this chapter. Where appropriate these constructs will remain in use for all subsequent derivations, but in some cases a different notation will be introduced within the nodal formalism in Chapter 3.

- Fluxes are defined at mesh centers, denoted by $\Phi_{s,t,u}$ within the region $r_s \leq r \leq r_{s+1}$, $z_t \leq z \leq z_{t+1}$, $\theta_u \leq \theta \leq \theta_{u+1}$. Note that mesh-edge fluxes could just as well have been chosen at this point, and would not impact on the accuracy, or computational efficiency of the method.
- $\bar{\Phi}_{s,t,u}$ denotes the mesh-averaged flux (note that this is different to the mesh centered flux above, although the assumption will shortly be made that these quantities are equal for sufficiently small meshes).
- $J_{s,t,u,\pm}^v$ denotes the side-averaged net current (in the direction of the outward unit normal) for each mesh (s, t, u) at the right (+) or left (-) side in the given direction $v = \{r, \theta, z\}$.
- $\sigma_{s,t,u}^{rem}$ denotes the mesh average macroscopic removal cross-section within mesh (s, t, u) . Note that $\sigma_{s,t,u}^{g,rem} = \sigma_{s,t,u}^{g,total} - \sigma_{s,t,u}^{g \rightarrow g,scat}$.
- $D_{s,t,u}$ denotes the diffusion coefficient within mesh (s, t, u) and $Q_{s,t,u}$ the source term within the mesh (s, t, u) . $Q_{s,t,u}$ will be expanded upon later in the text, but represents a combination of all possible sources for the current energy group.
- $\tilde{D}_{s,t,u,\pm}^v$ denotes the average mesh-edge diffusion coefficient of mesh (s, t, u) on the right (+) or left (-) side in direction $v = \{r, \theta, z\}$.
- $V_{s,t,u} = \frac{1}{2}(r_{s+1}^2 - r_s^2) \Delta z_t \Delta \theta_u$ represents the volume of mesh (s, t, u) .
- $S_{s,t,u,\pm}^v$ denotes the cylindrical surface area of mesh (s, t, u) on right (+) or left (-) side in direction $v = \{r, \theta, z\}$.
- $L_{s,t,u,\pm}^v$ denotes the leakage from mesh (s, t, u) across right (+) or left (-) surface in direction $v = \{r, \theta, z\}$.

2.3 Finite-difference equations in 3D cylindrical coordinates

We return to the problem formulation in Section 1.2, and recall that the diffusion eq. (1.1) was integrated over each mesh to yield the neutron balance equation (eq. (1.2)). We begin by examining this process in more detail.

The balance equation

Let us start again with the within-group diffusion equation, but in this case consider a system with cross-sections and diffusion coefficient which are spatially constant within a given discretized mesh (s, t, u) (as compared to eq. (1.1))

$$-D_{s,t,u} \nabla^2 \Phi(r, z, \theta) + \sigma_{s,t,u}^{rem} \Phi(r, z, \theta) - Q(r, z, \theta) = 0 \quad (2.1)$$

Note that the group index g is not present, and eq. (2.1) represent the within-group neutron diffusion equation. If we integrate eq. (2.1) over mesh (s, t, u) , the following balance relation for mesh (s, t, u) is obtained:

$$-\sum_{u=\{r,\theta,z\}} \int_{S_{s,t,u,\pm}^v} \tilde{D}_{s,t,u,\pm}^v [\vec{n} \cdot \nabla \Phi(r, z, \theta)] dS_{s,t,u,\pm}^v - Q_{s,t,u} V_{s,t,u} + \sigma_{s,t,u}^{rem} \Phi_{s,t,u} V_{s,t,u} = 0 \quad (2.2)$$

Based upon eq. (2.2), we may define:

- $-\tilde{D}_{s,t,u,\pm}^v [\vec{n} \cdot \nabla \Phi(r, z, \theta)]$, denoted by $J_{s,t,u,\pm}^v$, as the net current in the direction of the outward pointing unit normal vector $\vec{n}$, across each surface $S_{s,t,u,\pm}^v$ bounding volume $V_{s,t,u}$. Note that due to the application of the divergence theorem to eq. (2.1), there is a specific need for a surface-averaged diffusion coefficient $\tilde{D}_{s,t,u,n}^v$.
- $-\int_{S_{s,t,u,\pm}^v} \tilde{D}_{s,t,u,n}^v [\vec{n} \cdot \nabla \Phi(r, z, \theta)] dS_{s,t,u,\pm}^v$ as the leakage $L_{s,t,u,\pm}^v$ across each surface $S_{s,t,u,\pm}^v$ bounding volume $V_{s,t,u}$.
- $\tilde{D}_{s,t,u,\pm}^v$ as the mesh-edge diffusion coefficient on the surface, which still remains to be defined. Diffusion coefficients are supplied and are constant within each mesh, but some approximate inter-mesh averaged edge diffusion coefficient will have to be defined for use in eq. (2.2).
- $Q_{s,t,u}^g = q_{s,t,u}^{fixed} + \frac{1}{k_{eff}} \chi^g \sum_{h=1}^G v^h \sigma_f^h \Phi_{s,t,u}^h + \sum_{h=1, h \neq g}^G \Phi_{s,t,u}^h \sigma_{scat}^{h \rightarrow g}$ as the mesh source term,

which will be handled as constant within the in-group problem, and later coupled via an iteration scheme. The terms within this source term definition assume their usual meaning within the domain of reactor analysis methods, and the reader is referred to [3] for further description.

- Note that the assumption has now also been made that the mesh-averaged flux is equal to the mesh-centered flux. Thus:

$$\bar{\Phi}_{s,t,u} = \Phi_{s,t,u} \quad (2.3)$$

From this point onwards we will denote the mesh-averaged flux by $\Phi_{s,t,u}$. Rewriting eq. (2.2), we obtain:

$$\sum_{v=\{r,\theta,z\}} J_{s,t,u,\pm}^v S_{s,t,u,\pm}^v + \sigma_{s,t,u}^{\text{rem}} \Phi_{s,t,u} V_{s,t,u} = Q_{s,t,u} V_{s,t,u} \quad (2.4)$$

Eq. (2.4) describes the sources and sinks for neutrons for a given mesh (s, t, u) . The summation term refers to the net currents crossing the six surfaces of the mesh, the second term to the removal of neutrons through absorption or scattering to a different group and the right hand side to the source term, potentially consisting of in-scattering, fission and possible fixed sources within the mesh.

Application of the finite-difference approximation

Examining eq. (2.4) we notice that a further relationship is required between the mesh-averaged flux and the net current, and in this chapter we choose to resolve this issue by approximating the current by a finite-difference approximation. The finite-difference approximation is used to discretize the continuous gradient operator in eq. (2.2). Therefore, starting with our expression for leakage in eq. (2.2), applying the finite-difference approximation and explicitly writing it for the outer radial boundary of mesh (s, t, u) as illustration, we find

$$\begin{aligned} L_{s,t,u,+}^r &= \int_{S_n} J_{s,t,u,+}^r dS_n = - \int_{S_{(s,t,u,+)}^r} \widetilde{D}_{s,t,u,+}^r [\vec{n} \bullet \nabla \Phi(r, z, \theta)] dS_{s,t,u,+}^r \\ &= - \int_{S_{(s,t,u,+)}^r} \widetilde{D}_{s,t,u,+}^r \left[\frac{\partial}{\partial r} \Phi(r, z, \theta) \right] dS_{s,t,u,+}^r \\ &= - \int_{S_{(s,t,u,+)}^r} \widetilde{D}_{s,t,u,+}^r \left(\frac{\Phi_{s+1,t,u} - \Phi_{s,t,u}}{\frac{1}{2}(\Delta r_s + \Delta r_{s+1})} \right) dS_{s,t,u,+}^r \end{aligned} \quad (2.5)$$

In the same way the net currents on both sides in all directions may be approximated by such a finite-difference expression. Although easy to implement, such an approach does limit the mesh size quite severely due to the nature of the gradient approximation. It is further also clear from eq. (2.2) that the mesh-edge diffusion coefficient must still be defined. We must determine the edge diffusion coefficient, $\tilde{D}_{s,t,u,\pm}^v$, $v = \{r, \theta, z\}$, so that flux and current continuity are maintained within the finite-difference approximation. To solve this problem, we introduce redundant side fluxes $\Phi_{s+1,t,u}^-$ and $\Phi_{s,t,u}^+$, which refer to fluxes at left and right mesh-edges. If we use these fluxes to express continuity of currents at the right radial surface of mesh (s, t, u) , and left radial surface of mesh $(s+1, t, u)$, we find:

$$J_{s,t,u,+}^r = -D_{s,t,u}^r \frac{\Phi_{s+1,t,u}^- - \Phi_{s,t,u}^+}{\frac{1}{2}(\Delta r_s)} = J_{s+1,t,u,-}^r = -D_{s+1,t,u}^r \frac{\Phi_{s+1,t,u}^- - \Phi_{s+1,t,u}^+}{\frac{1}{2}(\Delta r_{s+1})} \quad (2.6)$$

Note that we have already enforced flux continuity by setting $\Phi_{s+1,t,u}^- = \Phi_{s,t,u}^+$ and that the mesh-centered diffusion coefficients $D_{s,t,u}^r$ are used within this finite difference approximation. By solving for the redundant flux, and replacing the solution into eq. (2.6), we find the current expression to be

$$J_{s,t,u,+}^r = -\tilde{d}_{s,t,u,+}^r [\Phi_{s+1,t,u} - \Phi_{s,t,u}] \quad (2.7)$$

where

$$\tilde{d}_{s,t,u,+}^r = \frac{2 \cdot d_{s,t,u}^r d_{s+1,t,u}^r}{d_{s,t,u}^r + d_{s+1,t,u}^r} \quad (2.8)$$

$$d_{s,t,u}^r = \frac{D_{s,t,u}^r}{\Delta r_s} \quad (2.9)$$

If we explicitly write the full expression for the averaged diffusion coefficient as

$$\tilde{D}_{s,t,u,+}^r = \frac{d_{s,t,u}^r d_{s+1,t,u}^r (\Delta r_s + \Delta r_{s+1})}{d_{s,t,u}^r + d_{s+1,t,u}^r} = \frac{(\Delta r_s + \Delta r_{s+1})}{\frac{\Delta r_s}{D_{s,t,u}^r} + \frac{\Delta r_{s+1}}{D_{s+1,t,u}^r}} \quad (2.10)$$

we find that the mesh-edge diffusion coefficient takes the form of the harmonic average of neighbouring mesh diffusion coefficients. For the generic coordinate directions v eq. (2.8) becomes for $v = r, z, \theta$ and $i = s, t, u$ respectively:

$$\tilde{d}_{i,\pm}^v = \frac{2 \cdot d_i^v d_{i\pm 1}^v}{d_i^v + d_{i\pm 1}^v} \quad (2.11)$$

$$\begin{aligned} d_i^r &= \frac{D_i}{\Delta r_i} \\ d_i^\theta &= \frac{D_i}{r_{mid} \Delta \theta} \\ d_i^z &= \frac{D_i}{\Delta z_i} \end{aligned} \quad (2.12)$$

We may now insert the new formulation of $J_{s,t,u,\pm}^v$ $\{v = r, z \text{ or } \theta\}$ into eq. (2.4), taking care to apply the process of eqs. (2.5-2.12) to each surface surrounding mesh (s, t, u) , namely two surfaces in the axial direction (bottom and top), two in the azimuthal direction (left and right) and two in the radial direction (inner and outer). If we explicitly expand the expressions, and for the moment describe only interior points, we obtain

$$\begin{aligned} & -\tilde{d}_{s,t,u,-}^r [\Phi_{s,t,u} - \Phi_{s-1,t,u}] r_s \Delta \theta_u \Delta z_t + \tilde{d}_{s,t,u,+}^r [\Phi_{s+1,t,u} - \Phi_{s,t,u}] r_{s+1} \Delta \theta_u \Delta z_t \\ & -\tilde{d}_{s,t,u,-}^\theta [\Phi_{s,t,u} - \Phi_{s,t,u-1}] \Delta r_s \Delta z_t + \tilde{d}_{s,t,u,+}^\theta [\Phi_{s,t,u+1} - \Phi_{s,t,u}] \Delta r_s \Delta z_t - \\ & -(-\tilde{d}_{s,t,u,-}^z [\Phi_{s,t,u} - \Phi_{s,t-1,u}] \Delta \theta_u (\frac{\Delta r_s^2}{2} + \Delta r_s r_s) + \tilde{d}_{s,t,u,+}^z [\Phi_{s,t+1,u} - \Phi_{s,t,u}] \Delta \theta_u (\frac{\Delta r_s^2}{2} + \Delta r_s r_s) \\ & -Q_{s,t,u} V_{s,t,u} + \sigma_{s,t,u}^{rem} \Phi_{s,t,u} V_{s,t,u} = 0 \end{aligned} \quad (2.13)$$

$$s = 1, 2 \dots N-2; t = 1, 2 \dots M-2; u = 1, 2 \dots P-2$$

The equation we obtained here is the discretized finite-difference form of eq. (2.4). This equation is rather tedious, but when expressed in terms of the surface areas

$$S_{s,t,u,-}^r = r_s \Delta \theta_u \Delta z_t$$

$$S_{s,t,u,+}^r = r_{s+1} \Delta \theta_u \Delta z_t$$

$$S_{s,t,u,-}^\theta = \Delta r_s \Delta z_t$$

$$S_{s,t,u,+}^\theta = \Delta r_s \Delta z_t$$

$$S_{s,t,u,-}^z = \Delta \theta_u (\frac{\Delta r_s^2}{2} + \Delta r_s r_s)$$

$$S_{s,t,u,+}^z = \Delta \theta_u (\frac{\Delta r_s^2}{2} + \Delta r_s r_s)$$

and finite-difference based surface-averaged currents

$$J_{s,t,u,-}^r = \tilde{d}_{s,t,u,-}^r [\Phi_{s,t,u} - \Phi_{s-1,t,u}]$$

$$J_{s,t,u,+}^r = -\tilde{d}_{s,t,u,+}^r [\Phi_{s+1,t,u} - \Phi_{s,t,u}]$$

$$J_{s,t,u,-}^\theta = \tilde{d}_{s,t,u,-}^\theta [\Phi_{s,t,u} - \Phi_{s,t,u-1}]$$

$$J_{s,t,u,+}^\theta = -\tilde{d}_{s,t,u,+}^\theta [\Phi_{s,t,u+1} - \Phi_{s,t,u}]$$

$$J_{s,t,u,-}^z = \tilde{d}_{s,t,u,-}^z [\Phi_{s,t,u} - \Phi_{s,t-1,u}]$$

$$J_{s,t,u,+}^z = -\tilde{d}_{s,t,u,+}^z [\Phi_{s,t+1,u} - \Phi_{s,t,u}]$$

we reconnect with the notation of eq. (2.4), now with currents defined as finite-difference relations):

$$\sum_v J_{s,t,u,\pm}^v S_{s,t,u,\pm}^v - Q_{s,t,u} V_{s,t,u} + \sigma_{s,t,u}^{rem} \Phi_{s,t,u} V_{s,t,u} = 0 \quad (2.14)$$

with $v = \{r, \theta, z\}$. We are now ready to reformulate the diffusion equation as a set of coupled linear equations, which may be solved via either direct inversion or standard matrix iterative methods.

2.4 3D solution process - the 7-point equations

Reformulating eq. (2.13) and grouping like flux terms, the following 7-point equations (linear system of equations, each with seven coupled unknowns) are obtained:

$$h_{s,t,u} \Phi_{s,t,u} - q_{s,t,u} \Phi_{s+1,t,u} - c_{s,t,u} \Phi_{s-1,t,u} - f_{s,t,u} \Phi_{s,t,u+1} - e_{s,t,u} \Phi_{s,t,u-1} - b_{s,t,u} \Phi_{s,t+1,u} - a_{s,t,u} \Phi_{s,t-1,u} - \quad (2.15)$$

$$k_{s,t,u} = 0$$

with:

$$c_{s,t,u} = \tilde{d}_{s,t,u,-}^r r_s \Delta z_t \Delta \theta_u$$

$$\begin{aligned}
q_{s,t,u} &= c_{s+1,t,u} \text{ with } \tilde{d}_{s+1,t,u,-}^r = \tilde{d}_{s,t,u,+}^r \\
e_{s,t,u} &= \tilde{d}_{s,t,u,-}^{\theta} - \frac{2\Delta z_1 \Delta r_s}{r_s + r_{s+1}} \\
f_{s,t,u} &= e_{s,t,u+1} \text{ with } \tilde{d}_{s,t,u+1,-}^{\theta} = \tilde{d}_{s,t,u,+}^{\theta} \\
a_{s,t,u} &= \tilde{d}_{s,t,u,-}^z - \Delta \theta_u \left(\frac{\Delta r_s^2}{2} + \Delta r_s r_s \right) \\
b_{s,t,u} &= a_{s,t+1,u} \text{ with } \tilde{d}_{s,t+1,u,-}^z = \tilde{d}_{s,t,u,+}^z \\
g_{s,t,u} &= \sigma_{s,t,u}^{rem} V_{s,t,u} \\
k_{s,t,u} &= Q_{s,t,u} V_{s,t,u} \\
h_{s,t,u} &= a_{s,t,u} + b_{s,t,u} + c_{s,t,u} + q_{s,t,u} + e_{s,t,u} + f_{s,t,u} + g_{s,t,u} \\
s &= 1, 2, 3, \dots, N-2; t = 1, 2, 3, \dots, M-2; u = 1, 2, 3, \dots, P-2
\end{aligned}$$

These expressions for the coupling coefficients, may be expressed in terms of surface areas:

$$\begin{aligned}
c_{s,t,u} &= \tilde{d}_{s,t,u,-}^r S_{s,t,u,-}^r \\
q_{s,t,u} &= c_{s+1,t,u} \\
e_{s,t,u} &= \tilde{d}_{s,t,u,-}^{\theta} S_{s,t,u,-}^{\theta} \\
f_{s,t,u} &= e_{s,t,u+1} \\
a_{s,t,u} &= \tilde{d}_{s,t,u,-}^z S_{s,t,u,-}^z \\
b_{s,t,u} &= a_{s,t+1,u} \\
g_{s,t,u} &= \sigma_{s,t,u}^{rem} V_{s,t,u} \\
k_{s,t,u} &= Q_{s,t,u} V_{s,t,u} \\
h_{s,t,u} &= a_{s,t,u} + b_{s,t,u} + c_{s,t,u} + q_{s,t,u} + e_{s,t,u} + f_{s,t,u} + g_{s,t,u} \\
s &= 1, 2, 3, \dots, N-2; t = 1, 2, 3, \dots, M-2; u = 1, 2, 3, \dots, P-2
\end{aligned} \tag{2.16}$$

The $(N-2) \times (M-2) \times (P-2)$ equations (2.16) in $(N \times M \times P)$ unknowns represent an open, simultaneous set, and require appropriate boundary conditions to close.

Boundary conditions

Boundary conditions will be formulated in a general way, using diagonal albedo matrices to allow user definable boundary conditions. To facilitate integration of the boundary conditions into the existing equation structure, the domain will be enlarged to $(N - 1)$ radial and M axial meshes. The albedo boundary condition will not be applied in the center of the cylinder (rather zero net current condition at $r = 0$), and therefore the radial domain is only enlarged at the outer boundary. Cyclic boundary conditions will be used in the azimuthal direction. The enlargement of the domain will allow fictitious $d_{s,t,u}^v$, $v = r, z$ or θ and $\Phi_{s,t,u}$ values to be defined in these outer zones, maintaining the existing equation structure for a more generic implementation. We would then be able to extend the index ranges of s, t and u in equation (2.16) and close the set. Note: Zero-flux boundary conditions can not be formulated using an albedo approach, and these have been implemented by adjusting coupling coefficients explicitly in the boundary meshes.

Radial boundary conditions

By using the definition of albedo $\alpha = \frac{J^-}{J^+}$, where $J^\pm$ refer to partial currents on a particular outer surface, as well as applying continuity of flux and current at mesh boundaries, outer radial boundary conditions in the fictitious outer zone may be formulated, as described in detail in [1], as:

$$d_{N,t,u}^r = \frac{1}{4} \frac{1 - \alpha_{outer}^r}{1 + \alpha_{outer}^r}$$

$$\Phi_{N,t,u} = 0$$

Having defined these unknowns in the boundary zones, eq. (2.11) may be used to extend the radial index in eq. (2.16) to run from 1 to $(N - 1)$. For implementation of the $r = 0$ zero net current condition, inspection of eqs. (2.13) and (2.16) shows that setting $c_{0,t,u} = 0$ in (2.16) will suffice. This allows the radial index s to further be extended to run from 0 to $(N - 1)$. In the case of zero-flux boundary conditions, setting the flux to zero at the outer boundary is equivalent to setting $q_{N-1,t,u} = 0$ and adding $\frac{2D_{N-1,t,u}}{\Delta r_N}$ to $h_{N-1,t,u}$ in eq. (2.16).

Azimuthal boundary conditions (Cyclic)

For implementation of the cyclic boundary conditions in the azimuthal direction, the following definitions are applied:

Starting angle boundary condition:

$$d_{s,t,0}^{\theta} = d_{s,t,P-1}^{\theta}$$

$$\Phi_{s,t,0} = \Phi_{s,t,P-1}$$

Final angle boundary condition:

$$d_{s,t,P-1}^{\theta} = d_{s,t,0}^{\theta}$$

$$\Phi_{s,t,P-1} = \Phi_{s,t,0}$$

Using these definitions, and eq. (2.11), the index u in eq. (2.16) may be extended to run from 0 to $(P - 1)$.

Axial boundary conditions

Similar to the outer radial boundary, the following boundary conditions are applied in the top and bottom fictitious axial zones:

Top zone:

$$d_{s,M,u}^z = \frac{1}{4} \frac{1 - \alpha_{outer}^z}{1 + \alpha_{outer}^z}$$

$$\Phi_{s,M,u} = 0$$

Bottom zone:

$$d_{s,-1,u}^z = \frac{1}{4} \frac{1 - \alpha_{inner}^z}{1 + \alpha_{inner}^z}$$

$$\Phi_{s,-1,u} = 0$$

Utilizing these definitions, eq. (2.11) may be used to extend the axial index t of eq. (2.16) to run from 0 to $M - 1$. In the case of zero-flux boundary conditions, setting the flux to zero at the outer boundaries is equivalent to setting:

- $a_{s,1,u} = 0$ and adding $\frac{2D_{s,0,u}}{\Delta z_0}$ to $h_{s,0,u}$ in (2.16) for the bottom boundary.
- $b_{s,M,u} = 0$ and adding $\frac{2D_{s,M,u}}{\Delta z_M}$ to $h_{s,M,u}$ in (2.16) for the top boundary.

Final form of 7-point equations

With the fictitious boundary fluxes and mesh-edge diffusion coefficients defined, eq. (2.16) may now be extended in its current form to include the entire domain, and form a closed set:

$$h_{s,t,u} \Phi_{s,t,u} - q_{s,t,u} \Phi_{s+1,t,u} - c_{s,t,u} \Phi_{s-1,t,u} - f_{s,t,u} \Phi_{s,t,u+1} - e_{s,t,u} \Phi_{s,t,u-1} - b_{s,t,u} \Phi_{s,t+1,u} - a_{s,t,u} \Phi_{s,t-1,u} - \quad (2.17)$$

$$k_{s,t,u} = 0$$

with:

$$c_{s,t,u} = \tilde{d}_{s,t,u}^r S_{s,t,u}^r -$$

$$q_{s,t,u} = c_{s+1,t,u}$$

$$e_{s,t,u} = \tilde{d}_{s,t,u}^\theta S_{s,t,u}^\theta -$$

$$a_{s,t,u} = \tilde{d}_{s,t,u}^z S_{s,t,u}^z -$$

$$b_{s,t,u} = a_{s,t+1,u}$$

$$f_{s,t,u} = e_{s,t,u+1}$$

$$g_{s,t,u} = \sigma_{s,t,u}^{rem} V_{s,t,u}$$

$$k_{s,t,u} = Q_{s,t,u} V_{s,t,u}$$

$$h_{s,t,u} = a_{s,t,u} + b_{s,t,u} + c_{s,t,u} + q_{s,t,u} + e_{s,t,u} + f_{s,t,u} + g_{s,t,u}$$

$$s = 0, 1, 2 \dots N-1; t = 0, 2 \dots M-1; u = 0, 1 \dots P-1$$

This represents a consistent formulation of the 7-point equations, since internal and boundary meshes are treated similarly.

2.4.1 Numerical implementation of solution

The set of equations presented in eq. (2.17), along with the described boundary conditions, can be written in matrix notation. Standard linear iterative methods may be applied to solve the system of $(N \times M \times P)$ equations, since the matrix is sparse, and direct methods would be highly inefficient. Ordering the unknowns lexicographically, (by traversing the problem domain azimuthally, then radially and finally axially) eq. (2.17) may be written as:

$$\mathbf{W}\mathbf{f} = \mathbf{r} \quad (2.18)$$

with $\mathbf{W}$ representing the $[N \times M \times P, N \times M \times P]$ coefficient matrix, $\mathbf{f}$ referring to the ordered $[N \times M \times P]$ vector of unknown fluxes, and $\mathbf{r}$ representing the source vector ($k_{s,t,u}$ in eq. (2.17)). The matrix produced will be sparse and diagonally dominant. Eq. (2.18) will be solved using a Gauss-Seidel iteration scheme, described below.

From eq. (2.17), the flux in mesh (s, t, u) may be expressed as follows:

$$\Phi_{s,t,u} = \frac{q_{s,t,u}\Phi_{s+1,t,u} + c_{s,t,u}\Phi_{s-1,t,u} + b_{s,t,u}\Phi_{s,t+1,u} + a_{s,t,u}\Phi_{s,t-1,u} + \frac{f_{s,t,u}\Phi_{s,t,u+1} + e_{s,t,u}\Phi_{s,t,u-1} + k_{s,t,u}}{h_{s,t,u}}}{h_{s,t,u}} \quad (2.19)$$

Since the fluxes on the right hand side are not known, the solution will be an iterative one, starting with an initial estimate for all fluxes and continuing until convergence criteria are reached. In our case, convergence will be measured by:

$$MAX_{s,t,u} \left| \frac{\Phi_{s,t,u}^{l+1} - \Phi_{s,t,u}^l}{\Phi_{s,t,u}^{l+1}} \right| < \lambda = 10^{-d} \quad (2.20)$$

where l denotes the iteration counter, and d the required number of significant digits in the allowable relative error. A further important factor to note is that the Gauss-Seidel iteration scheme makes use of new fluxes as they become available. Hence eq. (2.19) becomes:

$$\Phi_{s,t,u}^{l+1} = \frac{q_{s,t,u}\Phi_{s+1,t,u}^l + c_{s,t,u}\Phi_{s-1,t,u}^{l+1} + b_{s,t,u}\Phi_{s,t+1,u}^l + a_{s,t,u}\Phi_{s,t-1,u}^{l+1} + \frac{f_{s,t,u}\Phi_{s,t,u+1}^l + e_{s,t,u}\Phi_{s,t,u-1}^{l+1} + k_{s,t,u}}{h_{s,t,u}}}{h_{s,t,u}} \quad (2.21)$$

Starting with an initial guess for $\Phi_{s,t,u}^0$, eqs. (2.20) and (2.21) fully describe the Gauss-Seidel iteration scheme. Further acceleration can be achieved by applying the Successive Over Relaxation Method. In this case the flux is estimated as a weighted average between

the previous ($\Phi_{s,t,u}^l$) and current ($\Phi_{s,t,u}^{l+1}$) iteration solution, and utilizes a fixed relaxation parameter w (value typically in the order of 1.3). We therefore redefine $\Phi_{s,t,u}^{l+1}$ in eq. (2.21) as the intermediate quantity $\Phi_{s,t,u}^{l+\frac{1}{2}}$ and define the accelerated estimation of $\Phi_{s,t,u}^{l+1}$ as:

$$\Phi_{s,t,u}^{l+1} = \Phi_{s,t,u}^l + w(\Phi_{s,t,u}^{l+\frac{1}{2}} - \Phi_{s,t,u}^l) \quad (2.22)$$

Power Iteration scheme - eigenvalue problem solutions

The equations and solution methods described in this chapter are characterized as a within-group problem. For the sake of a multi-group problem, these equations will be extended to include a group index g . The solution will march through the groups, starting with the first fast energy group $g = 1$ and progressing up to a specified final thermal energy group index G .

An eigenvalue problem will be solved to include fissionable material within the source term Q , using a power iteration scheme. This scheme may be described as follows:

1. Choose a normalization for the total fission source F : $\int_V \sum_{h=1}^G v^h \sigma_f^h \Phi_{s,t,u}^h d^3r = \int_V F d^3r = V$, in other words normalize the fission source over the entire domain to the volume of the domain.
2. Begin with an initial guess for k_n and $F_{s,t,u}^n$, satisfying the chosen normalization. (n represents the new outer iteration counter vs. l which defines the inner Gauss Seidel iteration counter).
3. Solve the fixed source problem of eq. (1.2) as described in Section 2.3 to obtain $\Phi_{s,t,u}^{h,n+\frac{1}{2}}$ over all groups $h = 1$ to G , using $F_{s,t,u}^n$ for $\sum_{h=1}^G v^h \sigma_f^h \Phi_{s,t,u}^h$ in eq. (1.2).

4. Calculate

$$F_{s,t,u}^{n+\frac{1}{2}} = \sum_{h=1}^G v^h \sigma_f^h \Phi_{s,t,u}^{h,n+\frac{1}{2}}$$

5. Calculate

$$k^{n+1} = k^n \frac{\int_V F_{s,t,u}^{n+\frac{1}{2}} d^3r}{\int_V F_{s,t,u}^n d^3r}$$

6. Normalize the new fission source $F_{s,t,u}^{n+1} = \frac{F_{s,t,u}^{n+\frac{1}{2}}}{\frac{1}{V} \int_V F_{s,t,u}^{n+\frac{1}{2}} d^3r}$

7. Continue the process until convergence criteria are met for k , as well as convergence for the flux or fission source. In other words:

$$\left\| \frac{k^{n+1} - k^n}{k^{n+1}} \right\| \leq \frac{\varepsilon}{10}$$

and

$$\left\| \frac{F(r)^{n+1} - F(r)^n}{F(r)^{n+1}} \right\| \leq \varepsilon = 10^{-4}$$

where $\|\bullet\|$ denotes the magnitude of a quantity.

For a problem with no upscattering, such a solution method only iterates over the fission source. If upscatter from lower thermal groups is included, nested Gauss-Seidel iterations on the scattering source are used.

2.5 Code implementation and testing

The procedure described above was implemented by the author in a stand-alone FORTRAN code named **SciFi**. SciFi (neglecting the obvious acronymic description) is a 3D cylindrical, finite-difference, multi-group, eigenvalue and fixed source solution implementation, making use of macroscopic cross-section input. **SciFi** solves eq. (2.17), utilizing the numerical iteration schemes in Section 2.4.1. The most important results obtained from the code is the three-dimensional multi-group flux distribution, as well as the system multiplication factor or k_{eff} .

No explicit symmetry has been built into the code, and input must always be given as if for an (r, z, θ) problem. In order to perform 1D and 2D calculations at least one zone in the unused dimensions must still be defined and surrounded by fitting boundary conditions. E.g. if an infinite cylinder calculation is to be done, at least one axial zone has to be specified, and associated zero net current (reflective) boundary conditions used. The code does however allow for performing an azimuthal segment calculation, since periodic boundary conditions are implemented in the azimuthal direction. The full input manual specification of SciFi is given in Appendix A.

The SciFi code was further extended to include SP2 [20] and continuous P1-SP2 [21] transport corrections. Although these additions fall outside the scope of this thesis, the work is novel and was published in [24].

The SciFi code has been verified against various problems, and the results are summarized in this section. Comparisons were done and results compared with:

- An analytic infinite cylinder eigenvalue solution.

- a fixed source problem defined in [6],
- an eigenvalue problem defined in [7] and fully described in Appendix B.

Analytic infinite cylinder solution

The flux solution of a critical ($k_{eff} = 1$), axially infinite, homogeneous cylinder may be calculated analytically and written in terms of a zeroth order Bessel function of the first kind in the following way:

$$\phi(r) = J_0\left(\frac{\alpha_0 r}{R}\right)$$

where the geometric dimension is determined by equating material and geometric buckling, as described in [3], to maintain the critical condition ($k_{eff} = 1$) for the cylinder:

$$\left(\frac{\alpha_0}{R}\right)^2 = \frac{v\sigma_f - \sigma_a}{D}$$

Symbols have their usual meaning with R referring to the outer radius of the cylinder and α_0 to the first zero of the Bessel function ≈ 2.40482556 . In comparison, SciFi was run using the following criteria, and produced the correct k_{eff} value to within an accuracy of 0.2 pcm ($1 \text{ pcm} = \frac{\Delta k}{k} 10^{-5}$):

Parameter	Value
Radial meshes (equi-distant)	1 (200 times refined)
Axial meshes	1
Azimuthal meshes	1
Energy groups	1
Radial dimension	2.40482556 cm
Top and bottom boundaries	Reflective
Outer radial boundary	Zero-Flux
Convergence criteria	1×10^{-8}
<u>Cross-sections</u>	
Diffusion coefficient ($D_{s,t,u}$)	0.33 cm
Removal ($\sigma_{s,t,u}^{rem}$)	0.50 / cm
NuFission ($v\sigma_f$)	0.83 / cm
Self Scatter ($\sigma_{s,t,u}^{scat}$)	0.50 / cm
K-eff from SciFi	1.0000016 (0.2 pcm error)

Table 2.1: Description and result of an infinite homogeneous cylinder

In the case of this verification problem we were not interested in the full flux solution, but purely in the verification of the analytic eigenvalue solution (reproducing $k_{eff} = 1$). We conclude that the result obtained in Table 2.1, namely an eigenvalue accuracy within 0.2 pcm, shows that the power iteration scheme within SciFi is correctly implemented. For a more detailed flux solution verification, we proceed to the next comparison, and specifically with the fixed source problem described in [6].

Fixed source benchmark

The second comparison was done with a published one-group fixed source benchmark problem [6], which includes results from the Exterminator II finite-difference code system. This one-group (r, z) problem is geometrically specified below (the results are compared to extrapolated finite-difference results):

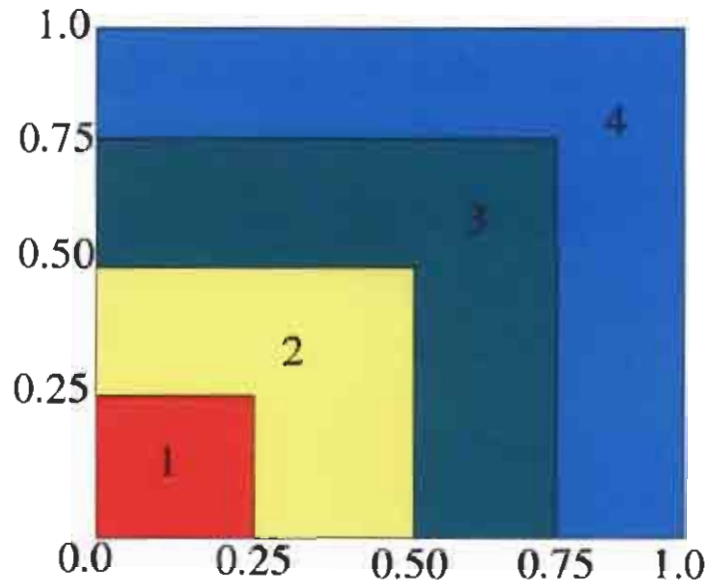


Figure 2.1: Azmi's (r, z) fixed source benchmark problem illustration

This cylindrical problem is specified with axial and outer radial zero-flux boundary conditions. Figure 2.1 represents a finite, four zone, inhomogeneous cylinder (the y-axis refers to the axial- and the x-axis to the radial coordinate), with the origin at its center. The figure presents an axial top-half symmetry segment of the problem, and may therefore be interpreted as four cylinders within each other. Table 2.2 further describes the problem

by providing cross-sections for each zone (1 to 4), as well as by comparing results for the volume-averaged fluxes in each zone.

Parameter	Zone 1	Zone 2	Zone 3	Zone 4
Absorption (1/cm)	400	100	36	25
Diffusion (cm)	1	1	1	1
Source (neutrons/cm ³)	1.0	0.0	0.0	0.0
Radial Meshing	10	10	10	10
Axial Meshing	10	10	10	10
Azimuthal Meshing	1	1	1	1
Radial Dimensions (cm)	0.25	0.25	0.25	0.25
Axial dimensions (cm)	0.25	0.25	0.25	0.25
<u>Results</u>				
Average Flux - extrapolated reference	1.98E-03	2.68E-04	2.04E-05	2.43E-06
Average Flux - SciFi (40x40)	1.99E-03	2.63E-04	2.03E-05	2.42E-06
Average Flux - CITATION	1.99E-03	2.62E-04	2.03E-05	2.42E-06
Axial Leakage - extrapolated ref				3.337E-05
Axial Leakage - SciFi				3.331E-05
Radial Leakage - extrapolated ref				1.014E-04
Radial Leakage - SciFi				1.022E-04

Table 2.2: Azmi's fixed source (r, z) verification problem

We may conclude that the obtained agreement between SciFi and both the CITATION and extrapolated published results, are within acceptable margins (less than 1% in zone averaged flux), and that the fixed source functionality in SciFi is correctly implemented.

2 Group eigenvalue solution - DODDS' benchmark

The DODDS' benchmark is a fixed cross-section (r, z) cylindrical reactor (heavy-water moderated) core model, with top and bottom reflector and blanket region in the outer radial zones. The problem is illustrated in Figure 2.2 below, but a detailed problem description is provided in Appendix B.

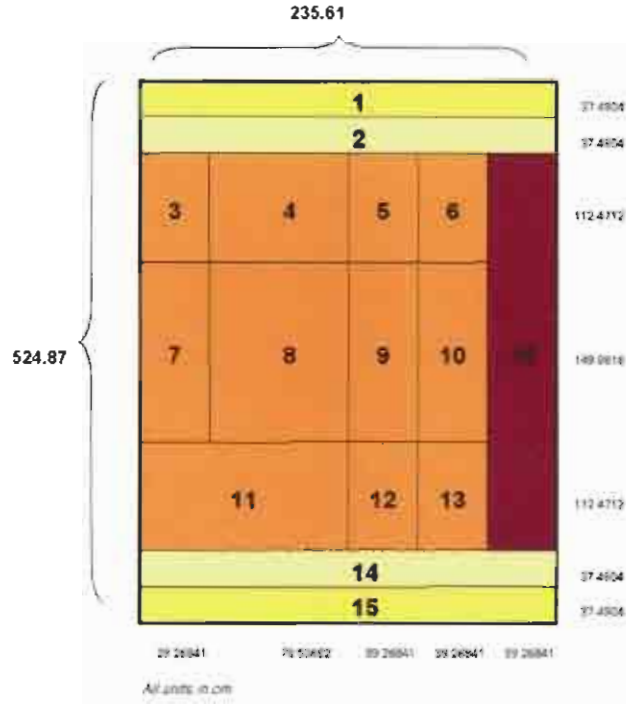


Figure 2.2: DODDS' benchmark model in (r, z) geometry

An independently published specification of the problem may be found in [7]. The published results are compared to the SciFi code using the input specification given in Appendix A. The results in Table 2.3 refer to coarse-mesh and fine-mesh solutions. Coarse-mesh indicates the benchmark meshing of $18 \text{ radial} \times 28 \text{ axial}$ meshes, and fine-mesh refers to a four-time refinement of the coarse meshing. In comparison, SciFi was run using the following criteria, and producing the following results:

Parameter	Value
Radial meshes (equi-volume)	18
Axial meshes	28
Azimuthal meshes	1
Energy groups	2
Radial dimension	235.6 cm
Axial dimension	524.87 cm
Top and bottom boundaries	Zero-Flux
Outer radial boundary	Zero-Flux
Convergence criterion	1×10^{-6}
Number of material types	9
Number of material regions	16
Results	
k_{eff} from Benchmark (coarse-mesh)	0.867053
k_{eff} from SciFi (coarse-mesh)	0.867053
k_{eff} from SciFi (fine-mesh - equi-distant)	0.866467
k_{eff} from SciFi (fine-mesh - equi-volume)	0.866468
k_{eff} from CITATION (coarse-mesh)	0.867005

Table 2.3: DODDS' benchmark description and results

Note that:

- The dimensions and discretization of DODDS' benchmark as listed in [7] (and in Figure 2.2 above) are not consistent with the results within that publication. Please refer to [8] for the correct material and dimensioning data. Material zone definitions were kept as are found in [7], but scaled to fit outer dimensions from [8].
- There is an error in the cross-section data as given in [7]. The diffusion coefficient in region 16 is 1.2997, and not 12.997 as indicated.
- All mentioned corrections are summarized in Appendix B.

From Table 2.3, we conclude that SciFi exactly reproduces the reference k_{eff} result from this problem (0.867053). This result is obtained with the exact coarse-mesh structure used in the benchmark problem. It is important to note that the true fine-mesh finite difference solution is somewhat different from this coarse mesh discretization result (400 pcm), and these fine-mesh results are given for two SciFi cases, namely equi-distant and equi-volume sub-mesh refinement. As independant confirmation of the benchmark result, the commercial

CITATION code is applied to the problem, and produces a result of 0.867005 (difference of 5 pcm). This small discrepancy is most probably associated with a somewhat non-standard implementation of zero-flux boundary conditions in CITATION and is not further elaborated upon here.

The input file for the DODDS⁸ benchmark problem, utilizing a radially equi-distant meshing, is included in Appendix C for illustration of the usage of the code.

2.6 Conclusion

SciFi showed good agreement, specifically eigenvalue accuracy within 1 pcm and flux accuracy within 1%, as compared to the chosen published results. Some components of the code system were not tested within the scope of the above benchmarks. These include azimuthal dependence, as well as multi-group upscattering problems. Examples featuring these requirements will be evaluated as part of the results and discussions in Chapter 6. This brings to an end the development of a cylindrical finite-difference test code for use as reference for the nodal test code to come. This cylindrical nodal method and associated code development, described in the next chapter, forms the backbone of this thesis, and signifies a new development within the field of full core reactor calculations.

Chapter 3

DERIVATION OF ANALYTIC NODAL METHOD IN CYLINDRICAL GEOMETRY

3.1 Introduction

Nodal diffusion methods [13] [10] have been used extensively in nuclear reactor core calculations, specifically for their performance advantage, but also for their superior accuracy. More specifically, the Analytic Nodal Method (ANM) [11] utilizing the transverse integration principle, has been applied to numerous reactor problems with much success [22]. Recent developments in the PBMR reactor project have sparked renewed interest in the application of different modeling methods to its design, and naturally included in this effort is a nodal method for cylindrical geometry.

The ANM is based on a transverse integration principle, resulting in a set of one-dimensional equations containing inhomogeneous sources. The issue of applying this method to 3D cylindrical geometry has never been satisfactorily addressed. Ougouag showed that the traditional transverse integration process fails in producing a one-dimensional equation in the θ -direction [12]. Instead, he suggested a two-dimensional solution in r and θ . This yields a set of equations that are analytically rather complex, and difficult to implement practically. In this chapter, a solution is proposed which entails the use of conformal mapping to circumvent these difficulties. This approach should yield a set of one-dimensional equations with an adjusted, geometrically dependent, inhomogeneous source. The concept of applying conformal mapping to simplify geometric complexity has been used with much success by Chao [16] to apply the ANM to hexagonal geometry, and the development in this

chapter signifies the first such effort with regard to cylindrical geometry reactor cores.

We will proceed by defining the nodal diffusion balance equation we wish to solve, and spend the greater part of this chapter on formulating the missing node-averaged flux to side-averaged current relationships needed within this balance equation. The latter part of the chapter will deal with representing the obtained relationships in a manageable form for use in a Fortran test code.

3.2 Balance equation in three dimensions

In order to sketch the problem we need to solve, we begin once more with the diffusion equation in three dimensions, and allow symbols to denote the same quantities as in Chapter 2 (eq. 2.1):

$$-D_n \nabla^2 \Phi^g(r, z, \theta) + \sigma_n^{g,rem} \Phi^g(r, z, \theta) - Q^g(r, z, \theta) = 0 \quad (3.1)$$

with

$$Q^g(r, z, \theta) = q^{fixed}(r, z, \theta)$$

for a fixed source problem, or

$$Q^g(r, z, \theta) = \frac{1}{k_{eff}} \chi^g \sum_{h=1}^G v^h \sigma_{fis,n}^h \Phi^h(r, z, \theta) + \sum_{h=1, h \neq g}^G \Phi^h(r, z, \theta) \sigma_{scat,n}^{h \rightarrow g}$$

in the case when the problem has multi-group scattering and/or fission source contributions.

We will however, solve this equation as a within-group problem, and therefore neglect the group index g in the coming derivation. In order to obtain a nodal balance relation, we integrate eq. (3.1) over each volume element n , denote the node number by subscript n , and node boundaries between node n and node j by subscript nj . We once more obtain the nodal balance relation, similar to eq. (2.2), but in this case maintaining the functional dependence in the intra-nodal flux $\Phi(r, \theta, z)$:

$$\sum_{j=1}^6 \bar{J}_{jn} S_{nj} - Q_n V_n + \sigma_n^{rem} \bar{\Phi}_n V_n = 0 \quad (3.2)$$

with

$$\bar{J}_{jn} = \frac{D_n}{S_{nj}} \frac{\partial}{\partial \vec{n}} \cdot \int_{S_{nj}} \Phi(r, \theta, z) dS_{nj} \quad (3.3)$$

$$\bar{\Phi}_n = \frac{1}{V_n} \int_{v_n} \Phi(r, \theta, z) dV_n \quad (3.4)$$

$$Q_n = \int_{v_n} Q(r, \theta, z) dV_n \quad (3.5)$$

where S_{nj} is the surface area between node n and node j , $\bar{J}_{jn}$ is the surface-averaged net current on surface nj in the direction of the outward unit normal and $\bar{\Phi}_n$ is the node-averaged flux of node n .

We proceed to divide eq. (3.2) with V_n to yield:

$$\sum_{j=1}^6 a_n^{nj} \bar{J}_{jn} + \sigma_n^{rem} \bar{\Phi}_n = Q_n \quad (3.6)$$

with

$$a_n^{nj} = \frac{S_{nj}}{V_n}$$

Note that the surface to volume ratios are different on opposite radial surfaces of node n . We reiterate that the description of the balance equation in eq. (3.6) is equivalent to the balance equation in Chapter 2 (eq. (2.2)), with the exceptions that all quantities in eq. (3.6) are divided by node volume, and that the intra-nodal flux and boundary currents have not been approximated.

Summative description of proposed solution

In eq. (3.6) we see that the surface-averaged currents and volume-averaged fluxes are the primary unknowns. We therefore need a further relationship to create a complete equation set. In order to find such a relationship we will apply a transverse integration procedure. We will integrate eq. (3.1) over all directions transverse to a chosen direction, to yield a one-dimensional equation in each of the coordinate directions. From each of these one-dimensional equations we may then obtain an analytic solution for the transverse integrated flux, and from there determine a relationship between volume-averaged flux and surface-averaged net currents in the chosen direction. Substituting these current-to-flux relationships back into the balance eq. (3.6) will yield a closed set of discretized equations.

This method of transverse integration works well in Cartesian coordinates [11] and can be directly applied in cylindrical geometry to obtain a one-dimensional equation in the z -direction. Some insurmountable difficulties, however, are experienced while performing the transverse integration procedure to obtain a one-dimensional θ equation. This mathematical

impasse is very clearly explained by Ougouag in [12]. An exercise in writing out the transverse integrated one-dimensional equations quickly show an inconsistency in defining transversely-averaged fluxes. The details hereof are referred to later in Section 3.4.2. To circumvent these difficulties, we introduce an extra step in order to obtain one-dimensional equations in the r and θ -directions. We firstly integrate the diffusion equation over the z direction to obtain a two-dimensional equation in the (r, θ) plane. Before we perform the second transverse integration, we will use conformal mapping to locally map a discretized cylindrical quadrilateral area element (or node) in the (r, θ) plane into a rectangular area element in the (u, v) plane, and then transversely integrate the resulting nodal equation in the rectangular coordinate.

The question must be asked why this transformation alone manages to circumvent the transverse integration problem encountered in the original (r, θ) coordinate system. In order to circumvent the transverse integration difficulty we will apply a “separation of variables” technique in the mapped Cartesian coordinate system. Although such an approximation is extremely restrictive within the original cylindrical coordinate system (the solution of the (r, θ) diffusion equation is not separable), it is proposed that the penalty is much less severe within the mapped Cartesian coordinate system. This statement will be proved numerically in this work, but future work may include a more rigorous analytic approach to this statement.

We proceed to solve the one-dimensional equations in each mapped direction, and obtain the needed surface-averaged current to node-averaged flux relationship in mapped coordinates. We transform the named relationship back to original cylindrical geometry before inserting the expressions for current back into the balance equation (eq. (3.6)).

We continue to solve the balance equation in cylindrical geometry, and obtain a solution in the original coordinate system. This conformal mapping technique is described in the next section. There is, of course, a penalty to pay for the simplification of the transverse integration process with conformal mapping. As will be seen, this penalty arises in the shape of an extra inhomogeneous “ghost” source introduced on the right hand side of the diffusion equation in both mapped directions. Later in this chapter some time will be spent on dealing with these ghost sources.

The approach very briefly described here sketches the flow of this chapter, and summarizes the ideas behind that which is new in this work. The chapter will elaborate in quite some detail upon each of the above paragraphs by

- performing the conformal mapping,
- relating the original and mapped coordinate systems,

- performing the transverse integration and handling the transverse leakage terms,
- solving the mapped one-dimensional equations and
- solving the cylindrical balance equation.

3.3 Conformal mapping

Mapping function

The technique of conformal mapping is a well-known matter arising from complex analysis and the reader is referred to [5] for a general overview of the topic and its properties. For the purpose of this application, the most important properties relating to conformal mapping are:

- the Laplacian operator in eq. (3.1) is invariant under conformal mapping.
- The mapping function from a cylindrical element to a rectangular element is given by a straight-forward analytic function. This is an advantage, since no numerical evaluation of the mapping function is required.

In this section we will apply the conformal mapping strategy to a local cylindrical area element in the complex plane Z ($Z = x + iy = re^{i\theta}$), and map it to a rectangular element in the complex plane W ($W = u + iv$). The mapping function which performs such a transformation is given by:

$$W = \text{Log}(Z) \quad (3.7)$$

Equating components in eq. (3.7) yields:

$$u + iv = \ln |Z| + i \text{Arg}(Z) \quad (3.8)$$

$$\therefore u = \ln(r) ; v = \theta$$

and

$$r = e^u$$

Node scaling

We intend to locally map the discretized domain defined by $0 < r \leq R_{outer}$ and $0 \leq \theta < 2\pi$. We will, however, be forced to exclude the center point at $r = 0$ from the mapping, since the logarithmic function exhibits a singularity at $r = 0$. Our approach to this exclusion will be to define a small ring at R_{inner} and normalize the domain to that point, thus excluding the zero point from our mapping. A boundary condition shall be placed at R_{inner} (or at 1 after normalization with R_{inner}). The mapping domain is therefore:

$$1 \leq r^{norm} \leq \frac{R_{outer}}{R_{inner}} \quad (3.9)$$

$$0 \leq \theta < 2\pi$$

We will use the conformal mapping technique to locally map a discretized cylindrical area element, in order to obtain a transversely integrated solution within that local node. Such a local area element is defined as follows:

$$r_i^{norm} \leq r^{norm} \leq r_{i+1}^{norm} \quad (3.10)$$

$$r_i^{norm} = \frac{r_i}{R_{inner}}$$

$$\theta_j \leq \theta < \theta_{j+1}$$

Applying eq. (3.7) to such a node will yield a transformed node with coordinates:

$$\ln(r_i^{norm}) \leq u_{node} \leq \ln(r_{i+1}^{norm}) \quad (3.11)$$

$$\theta_j \leq v < \theta_{j+1}$$

and dimensions $\{h_u, h_v\}$:

$$h_u = \ln(r_{i+1}) - \ln(r_i) = \ln\left(\frac{r_{i+1}}{r_i}\right) \quad (3.12)$$

$$h_v = \theta_{j+1} - \theta_j$$

From eq. 3.12 and onward we drop the radial superscript *norm*. Note that the radial coordinate is now dimensionless, since it was divided by the inner radius of the system. For

the rest of this derivation, R_{inner} will be assumed to be 1, and implemented in the test code as such. The mapping procedure is graphically represented in Figure 3.1:

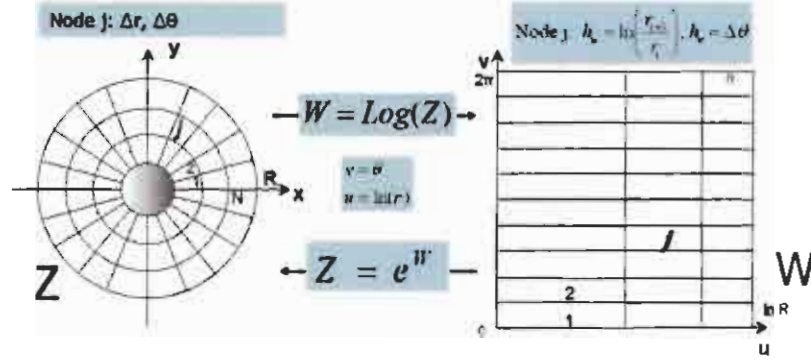


Figure 3.1: Conformal mapping - cylindrical to rectangular mapping

It illustrates the geometric relationship between the original and mapped coordinate systems. Furthermore, the figure graphically illustrates the logarithmically decreasing node sizes in the W plane versus the equi-distantly spaced radial node sizes in the Z plane. The largest mapped node sizes are found near the center. Note also the inner cut-out placed upon the mapping domain.

Since we will later represent functional expressions in terms of Legendre polynomials, it will be beneficial to obtain a symmetric node, i.e. $(-\frac{h_u}{2}, \frac{h_v}{2})$, after conformal mapping. To achieve this we scale the original radial node with scaling factor $\sqrt{r_i r_{i+1}}$ prior to mapping. This yields

$$r^{scal} = \frac{r}{\sqrt{r_i r_{i+1}}} \quad (3.13)$$

If we now return to the 3D diffusion equation in (3.1), we see that if we integrate eq. (3.1) over the z -direction, and then apply the mentioned radial normalizations, we remain with an equation purely in the (r^{scal}, θ) plane for node n , appropriately scaled so that the node is symmetric after mapping to (u, v) . The z -integrated equation takes the form:

$$-D_n \nabla^2 \Phi_z(r, \theta) + \sigma_n^{rcm} \Phi_z(r, \theta) = Q_{n,z}(r, \theta) - L_{r\theta}^z(r, \theta) \quad (3.14)$$

We may proceed to normalize the radial coordinate in the node using eq. (3.13):

$$-D_n \frac{1}{\eta^2} \nabla^2 \Phi_z(r^{scal}, \theta) + \sigma_n^{rcm} \Phi_z(r^{scal}, \theta) = Q_{n,z}(r^{scal}, \theta) - L_{r\theta}^z(r^{scal}, \theta) \quad (3.15)$$

with

$$\eta^2 = r_i r_{i+1}, \text{ and}$$

$$L_{r\theta}^z(r^{scal}, \theta) = \frac{-D_n}{h_z} \left[\frac{\partial}{\partial z} \Phi(r^{scal}, \theta, z) \right]_{-\frac{h_z}{2}}^{\frac{h_z}{2}}$$

$$\Phi_z(r^{scal}, \theta) = \frac{1}{h_z} \int_{h_z} \Phi(r^{scal}, \theta, z) dz$$

$$Q_{n,z}(r^{scal}, \theta) = \frac{1}{h_z} \int_{h_z} Q(r^{scal}, \theta, z) dz$$

h_z represents the node size in z - direction

In order to transform this equation with conformal mapping, we need to transform the differential operator as well and obtain:

$$\nabla^2(r, \theta) \Phi_z(r, \theta) = \frac{1}{e^{2u}} \nabla^2(u, v) \Phi_z(u, v)$$

The resulting mapped equation then takes the form

$$-D_n \frac{1}{r_i r_{i+1}} \left(\frac{\partial^2 \Phi_z(u, v)}{\partial u^2} + \frac{\partial^2 \Phi_z(u, v)}{\partial v^2} \right) + \sigma_n^{rem} \Phi_z(u, v) g(u)^2 = Q_{n,z}(u, v) g(u)^2 - L_{uv}^z(u, v) g(u)^2 \quad (3.16)$$

with

$$g(u)^2 = e^{2u} \text{ and denotes the area mapping function.}$$

The resulting mapped node is rectangular and its size is:

$$\left(\ln\left(\frac{r_i}{\sqrt{r_i r_{i+1}}}\right), \ln\left(\frac{r_{i+1}}{\sqrt{r_i r_{i+1}}}\right) \right) = \left(-\frac{\ln\left(\frac{r_{i+1}}{r_i}\right)}{2}, \frac{\ln\left(\frac{r_{i+1}}{r_i}\right)}{2} \right) = \left(-\frac{h_u}{2}, \frac{h_u}{2} \right) \quad (3.17)$$

After a translation of

$$\theta_j^t = \theta_j - \frac{\Delta\theta}{2}$$

the mapped v coordinate is:

$$(\theta_j, \theta_{j+1}) \rightarrow \left(-\frac{h_v}{2}, \frac{h_v}{2} \right) \quad (3.18)$$

3.3.1 Relationship between mapped and unmapped quantities

The concept of the coordinate transformation, or mapping, is now defined and we begin, in this section, by developing some critical relationships between important quantities in original cylindrical and mapped Cartesian coordinates.

The mapped coordinate system, as mentioned above, will only be used to perform the transverse integration process and obtain the required node-averaged flux to side-averaged current relationship. This relationship must then be mapped back to the original coordinate system and reinserted into the balance equation. To facilitate this “unmapping”, two primary quantities, namely the node-averaged flux and the side-averaged currents, must be related between the two coordinate systems. Let us therefore begin with this end in mind, and prior to completing the transverse integration process, define these critical relationships between the (r, θ) and (u, v) coordinate systems.

Node-averaged flux definition

The definition of node-averaged flux in the original coordinate system may be written in terms of a surface integral over the z -averaged flux (which was obtained in eq. (3.15)):

$$\bar{\Phi}_n = \frac{1}{S_n^{r\theta}} \int_{r\theta} \Phi_z(r, \theta) r dr d\theta \quad (3.19)$$

If we apply the radial scaling prior to mapping, then

$$\begin{aligned} \bar{\Phi}_n &= \frac{r_i r_{i+1}}{S_n^{r\theta}} \int_{r^{scal}\theta} \Phi_z(r^{scal}, \theta) r^{scal} dr^{scal} d\theta \\ &= \frac{1}{S_n^{r^{scal}\theta}} \int_{r^{scal}\theta} \Phi_z(r^{scal}, \theta) r^{scal} dr^{scal} d\theta \end{aligned} \quad (3.20)$$

The node-averaged flux in original and scaled coordinates are of course equal. Now applying the conformal mapping to this integral, ie.:

$$u = \ln(r^{scal}), \quad v = \theta$$

yields

$$\bar{\Phi}_n = \frac{r_i r_{i+1}}{S_n^{r\theta}} \int_{uv} \Phi_z(u, v) e^{2u} du dv \quad (3.21)$$

Notice that if we express the mapped node-averaged flux directly in terms of the (u, v) coordinate system, as per definition of a surface-averaged quantity, we would find that:

$$\bar{f}_n = \frac{1}{h_u h_v} \int_{uv} \Phi_z(u, v) du dv \quad (3.22)$$

We call this quantity the mapped node-averaged flux or simply the average one-dimensional flux, and strive to relate it to the node-averaged flux in the original coordinate system (relate eqs. 3.21 and 3.22).

Relationship between node-averaged flux and averaged one-dimensional flux (mapped average)

Eqs. (3.21) and (3.22) suggests that a relationship between one-dimensional average and original node-averaged flux may be found. We perform the v -integration and rescale the u variable to $(-1, 1)$ via $\xi = \frac{2u}{h_u}$ in equation (3.21). The node-averaged flux is then written as

$$\bar{\Phi}_n = \frac{K}{2} \int_{-1}^1 \Phi_{zv}(\xi) e^{2\xi} d\xi \quad (3.23)$$

where

$$K = \frac{h_u h_v r_{i+1}}{S_n^{\tau\ell}} \text{ (interpreted as ratio between scaled and mapped area)} \quad (3.24)$$

with

$$\xi = \frac{2u}{h_u}$$

Within this coordinate system, eq. (3.22) for the one-dimensional average flux may also be written, per definition, as:

$$\bar{f}_n = \frac{1}{2} \int_{-1}^1 \Phi_{zv}(\xi) d\xi$$

If we express, in eq. (3.23), the one-dimensional flux ($\Phi_{zv}(\xi)$) and the mapping function ($e^{2\xi}$) in terms of a Legendre polynomial expansion, we find:

$$e^{2\xi} = \sum_{l=0}^L g_l P_l(\xi) \text{ and } \Phi_{zv}(\xi) = \sum_{l=0}^L f_l^u P_l(\xi) \quad (3.25)$$

with

$$g_l = \frac{2l+1}{2} \int_{-1}^1 e^{2\xi} P_l(\xi) d\xi$$

$$f_l^u = \frac{2l+1}{2} \int_{-1}^1 \Phi_{zv}(\xi) P_l(\xi) d\xi$$

Here we have truncated infinite sums to a finite number of terms L . Employing these definitions, we express the node-averaged flux as:

$$\bar{\Phi}_n = K \sum_{l=0}^L \frac{g_l f_l^u}{2l+1} = \bar{f}_n + K \sum_{l=1}^L \frac{g_l f_l^u}{2l+1} \quad (3.26)$$

since

$$g_0 = \frac{\sinh(h_u)}{h_u} = \frac{\frac{r_{i+1}}{r_i} - \frac{r_i}{r_{i+1}}}{2h_u} = \frac{h_v(r_{i+1}^2 - r_i^2)}{2h_u h_v r_i r_{i+1}} = \frac{S_n^{r\theta}}{h_u h_v r_i r_{i+1}} = \frac{1}{K}$$

Eq. (3.26) is an important result, since it allows a clean expression for the node-averaged flux in terms of the mapped average flux (one-dimensional average) obtained from the transversely integrated equations. This relationship is the first of two which we need to relate the original and mapped coordinate system.

Side-averaged current definition

A second very important quantity which we will have to map between coordinate systems is the surface-averaged current. Using the net current definitions before and after mapping, we may relate mapped and unmapped currents on radial and azimuthal surfaces by:

$$J_{n,r}(r_n^-) = \frac{1}{r_n^-} J_{n,u}(-\frac{h_u}{2}) \quad (3.27)$$

$$J_{n,r}(r_n^+) = \frac{1}{r_n^+} J_{n,u}(+\frac{h_u}{2})$$

$$J_{n,\theta}(\theta_n^-) = \frac{h_{u,n}}{\Delta r_n} J_{n,v}(-\frac{h_v}{2})$$

$$J_{n,\theta}(\theta_n^+) = \frac{h_{u,n}}{\Delta r_n} J_{n,v}(+\frac{h_v}{2})$$

The above relationships in the θ -direction assume that the net currents across azimuthal surfaces have been appropriately averaged along the radial direction. This averaging produces the $\frac{h_{u,n}}{\Delta r_n}$ factor which would otherwise not be expected, since the azimuthal coordinate is not transformed during the mapping procedure.

3.4 Transverse integration of mapped equations

The basis for this approach has now been laid, and in order to proceed we have to develop the auxiliary one-dimensional equations in each direction, and solve them analytically to construct a balance relation which can be solved (in other words eq. (3.6) written in terms of node-averaged flux only). The ANM in Cartesian coordinates naturally makes use of the transverse integration process in order to obtain the auxiliary one-dimensional equations and this process, as applied to Cartesian geometry, is fully described by Smith in [11]. Nevertheless, due to the application of conformal mapping, some further complexities arise in the application of transverse integration to the mapped Cartesian geometry, and therefore this process is fully described here up until the end of Section 3.8.

We will now perform the first step of the transverse integration - firstly by integrating eq. (3.16) over v to find a one-dimensional equation in u , and thereafter over u to yield a one-dimensional equation in v . We also obtain a one-dimensional equation in the z -direction by transversely integrating the cylindrical diffusion equation (3.1) over r and θ directions. We then solve these one-dimensional equations in u , v and z analytically to obtain the required relationships between volume-averaged flux and surface-averaged currents in each direction.

3.4.1 Transverse integration over v : the u -equation

We begin by integrating equation (3.16) over v . We apply the integral:

$$\frac{1}{h_v} \int_{-\frac{h_v}{2}}^{\frac{h_v}{2}} \cdot dv$$

and find

$$-\frac{1}{\eta^2} D \frac{d^2}{du^2} f_n(u) + \sigma_n^{rem} g(u)^2 f_n(u) = g(u)^2 Q_n(u) - L_{n,u}(u) \quad (3.28)$$

where

$$f_n(u) = \frac{1}{h_v} \int_{h_v} \Phi_z(u, v) dv$$

$$Q_n(u) = \frac{1}{h_v} \int_{h_v} Q_z(u, v) dv$$

$$L_{n,u}(u) = \frac{1}{\eta^2} L_{n,u}^v(u) + g(u)^2 L_{n,u}^z(u)$$

$$L_{n,u}^v(u) = \frac{-D_n}{h_v} \left[\frac{\partial}{\partial v} \Phi_z(u, v) \right]_{-\frac{h_v}{2}}^{\frac{h_v}{2}} = \frac{J_v(u, \frac{h_v}{2}) + J_v(u, -\frac{h_v}{2})}{h_v}$$

$$L_{n,u}^z(u) = \frac{1}{h_v} \int_{h_z} \frac{-D_n}{h_z} \left[\frac{\partial}{\partial z} \Phi(u, v, z) \right]_{-\frac{h_z}{2}}^{\frac{h_z}{2}} dv = \frac{J_z(u, \frac{h_z}{2}) + J_z(u, -\frac{h_z}{2})}{h_z}$$

We move the inhomogeneous components to the right hand side and find:

$$-\frac{1}{\eta^2} D \frac{d^2}{du^2} f_n(u) + \sigma_n^{rem} f_n(u) = g(u)^2 Q_n(u) + s_n(u) - L_{n,u}(u) = R_{n,u}(u) \quad (3.29)$$

where

$$s_n(u) = (1 - g(u)^2) \sigma_n^{rem} f_n(u)$$

Eq. (3.29) is now an ordinary inhomogeneous linear differential equation, which may be solved analytically (assuming that we know the right hand side).

Summary term analysis of the u -equation

In order to solve eq. (3.29) we express the inhomogeneous sources on the right hand side in terms of Legendre polynomial expansions. The details of the one-dimensional solution, and exact formulation of these expansions will be described in Section 3.5, but for completeness some notation and formalism will be introduced here.

1. $L_{n,u}^z(u)$ and $L_{n,u}^v(u)$ represent the transverse leakage terms and will be expressed as Legendre polynomials: $L_{n,u}(u) = \sum_{l=0}^L l_l^u P_l(\frac{2u}{h_u})$. These expansions are developed in Section 3.9.

2. $s_n(u) = (1 - g(u)^2) \sigma_n^{rem} f_n(u) = \sum_{l=0}^L s_l^u P_l(\frac{2u}{h_u})$. These moments will be expressed as two terms:

$$s_l^u = \frac{2l+1}{h_u} \int_{h_u} (1 - g(u)^2) \sigma_n^{rem} f_n(u) P_l(\frac{2u}{h_u}) du.$$

$$s_l^u = \frac{\sigma_n^{rem} (2l+1)}{h_u} \left(\int_{h_u} f_n(u) P_l(\frac{2u}{h_u}) du - \int_{h_u} g(u)^2 f_n(u) P_l(\frac{2u}{h_u}) du \right)$$

The first integral term will be classified as **flux moments**, the second as **mapped flux moments**. These expressions will be developed in Section 3.5.1.

3. $g(u)^2 Q_n(u) = \sum_{l=0}^L q_l^u P_l(\frac{2u}{h_u})$ with $q_l^u = \frac{2l+1}{h_u} \int_{h_u} g(u)^2 Q_n(u) P_l(\frac{2u}{h_u}) du$. These source moment expressions will utilize the flux moments also (in the case of fission and scattering sources), but will further require moments of the mapping function. These expressions are also developed in Section 3.5.1.

Using these expansions we may express the right hand side of eq. (3.29) in terms of Legendre polynomials:

$$R_{n,u}(u) = \sum_{l=0}^L d_l^u P_l(\frac{2u}{h_u}) \quad (3.30)$$

$$d_l^u = q_l^u + s_l^u - l_l^u$$

3.4.2 Transverse integration over u : the v -equation

We proceed in a similar fashion by integrating equation (3.16) over u . We apply the integral

$$\frac{1}{h_u} \int_{-\frac{h_u}{2}}^{\frac{h_u}{2}} \cdot du$$

This process yields

$$-\frac{1}{\eta^2} D \frac{d^2}{dv^2} f_n(v) + \sigma_n^{\text{rem}} \Phi_{z,u}(v) = Q_n(v) - L_{n,v}(v) = R_{n,v}(u) \quad (3.31)$$

with

$$f_n(v) = \frac{1}{h_u} \int_{h_u} \Phi_z(u, v) du$$

$$Q_n(v) = \frac{1}{h_u} \int_{h_u} g(u)^2 Q_z(u, v) du$$

$$\Phi_{z,u}(v) = \frac{1}{h_u} \int_{h_u} g(u)^2 \Phi_z(u, v) du$$

$$L_{n,v}(v) = \frac{1}{\eta^2} L_{n,v}^u(v) + L_{n,v}^z(v)$$

$$L_{n,v}^u(v) = \frac{-D_n}{h_u} \left[\frac{\partial}{\partial u} \Phi_z(u, v) \right]_{-\frac{h_u}{2}}^{\frac{h_u}{2}} = \frac{J_u(\frac{h_u}{2}, v) + J_u(-\frac{h_u}{2}, v)}{h_u}$$

$$\begin{aligned}
L_{n,v}^z(v) &= \frac{1}{h_u} \int_{h_u} g(u)^2 \frac{-D_n}{h_z} \left[\frac{\partial}{\partial z} \Phi_z(u, v, z) \right]_{-\frac{h_z}{2}}^{\frac{h_z}{2}} du \\
&= \frac{\int_{h_u} g(u)^2 J_z(u, v, \frac{h_z}{2}) du + \int_{h_u} g(u)^2 J_z(u, v, -\frac{h_z}{2}) du}{h_z}
\end{aligned}$$

It is important to notice that we deal, in this equation, with a troublesome issue. Firstly we find two different definitions for the u -averaged flux, namely $\Phi_{z,u}(v)$ and $f_n(v)$, which represent the one-dimensional flux in original and mapped coordinates, respectively. This is a similar “impasse” found by Ougouag in [12], with the difference that we face this problem from the perspective of the one-dimensional diffusion equation in Cartesian, and no longer cylindrical, geometry. In order to circumvent this issue, we firstly perform the following manipulation of the one-dimensional flux by expanding the mapping function onto a Legendre polynomial base:

$$\begin{aligned}
\Phi_{z,u}(v) &= \frac{1}{h_u} \int_{h_u} g(u)^2 \Phi_z(u, v) du = \frac{1}{h_u} \int_{h_u} \sum_{l=0}^{\infty} g_l P_l\left(\frac{2u}{h_u}\right) \Phi_z(u, v) du \\
&= \frac{f(v)}{K} + \frac{1}{h_u} \int_{h_u} \sum_{l=1}^{\infty} g_l P_l\left(\frac{2u}{h_u}\right) \Phi_z(u, v) du
\end{aligned}$$

Here we defined the Legendre moments of the mapping function as

$$g_l = \frac{2l+1}{h_u} \int_{-\frac{h_u}{2}}^{\frac{h_u}{2}} e^{2u} P_l\left(\frac{2u}{h_u}\right) du$$

The same approach is used for the two-dimensional source term definition by writing

$$\begin{aligned}
Q_n(v) &= \frac{1}{h_u} \int_{h_u} g(u)^2 Q_z(u, v) du = \frac{1}{h_u} \int_{h_u} \sum_{l=0}^{\infty} g_l P_l\left(\frac{2u}{h_u}\right) Q_z(u, v) du \\
&= \frac{q(v)}{K} + \frac{1}{h_u} \int_{h_u} \sum_{l=1}^{\infty} g_l P_l\left(\frac{2u}{h_u}\right) Q_z(u, v) du
\end{aligned}$$

with

$$q_n(v) = \frac{1}{h_u} \int_{h_u} Q_z(u, v) du$$

With these expansions terminated at some fixed order L , eq. (3.31) may be rewritten as:

$$-\frac{1}{\eta^2} D \frac{d^2}{dv^2} f_n(v) + \frac{\sigma_n^{\text{rem}}}{K} f_n(v) = s_n(v) + Q_n(v) - L_{n,v}(v) \quad (3.32)$$

Here we have managed to successfully complete the transverse integration, and group the problematic functional forms into the right-hand-side sources, specifically

$$s_n(v) = -\sigma_n^{\text{rem}} \frac{1}{h_u} \int_{h_u} \sum_{l=1}^L g_l P_l\left(\frac{2u}{h_u}\right) \Phi_z(u, v) du \quad (3.33)$$

and

$$Q_n(v) = \frac{q_n(v)}{K} + \frac{1}{h_u} \int_{h_u} \sum_{l=1}^L g_l P_l\left(\frac{2u}{h_u}\right) Q_z(u, v) du \quad (3.34)$$

This formulation is the first important milestone in circumventing the transverse integration problem described by Ougouag in [12]. The problem has now been reduced to handling the non-linear source terms in eqs. (3.33) and (3.34).

The higher order terms in expressions (3.33) and (3.34) require some special treatment, and in these cases the assumption of separation of variables leads to relatively manageable constructions. The validity of these assumptions are not obvious, and will be numerically evaluated in later chapters. Assuming such an approach, two choices are available. These concern the form of the separation of variables, either as a sum or a product, of two one-dimensional solutions. The next four sections develop these approaches.

Summed variable separation - inhomogeneous source

In this instance, variable separation is assumed in the following form:

$$\Phi_z(u, v) = f_n(u) + f_n(v) - \bar{f} \quad (3.35)$$

where

$$f_n(v) = \frac{1}{h_u} \int_{h_u} \Phi_z(u, v) du$$

$$f_n(u) = \frac{1}{h_v} \int_{h_v} \Phi_z(u, v) dv$$

$$\bar{f} = \frac{1}{h_u h_v} \int_{h_u h_v} \Phi_z(u, v) dv du$$

This approximation is necessary in order to complete the transverse integration procedure. In short, the motivation is based upon the fact that the solution of the homogeneous diffusion equation in Cartesian coordinates is separable, but not so in cylindrical coordinates. It is reiterated that this approximation will be evaluated numerically, and future work will

include a rigorous analysis of the error inherent to this approach. Applying this approach to the inhomogeneous source term $s_n(v)$ (eq. 3.33) yields:

$$s_n(v) = -\sigma_n^{\text{rem}} \frac{1}{h_u} \int_{h_u} \sum_{l=1}^L g_l P_l\left(\frac{2u}{h_u}\right) (f_n(u) + f_n(v) - \bar{f}) du$$

Notice that the contributions from the $f_n(v)$ and $\bar{f}$ terms are zero, since the summation counts from 1. Thus, the expression for the inhomogeneous source term may be reduced as follows:

$$s_n(v) = \frac{-\sigma_n^{\text{rem}}}{h_u} \int_{h_u} \sum_{l=1}^L g_l P_l\left(\frac{2u}{h_u}\right) f_n(u) du = -\sigma_n^{\text{rem}} \sum_{l=1}^L \frac{g_l f_l^u}{2l+1} \quad (3.36)$$

where we define the Legendre moments of the one-dimensional flux in u -direction as follows:

$$f_l^u = \frac{2l+1}{h_u} \int_{h_u} f_n(u) P_l\left(\frac{2u}{h_u}\right) du$$

Note that this expression is actually constant in v , and this fact results from the summative separation approximation.

Summative variable separation - standard source term

We also approximate the standard (fission and scattering) source term in the same way by writing

$$Q(u, v) = Q_n(u) + Q_n(v) - \bar{Q} \quad (3.37)$$

$$Q_n(v) = \frac{1}{h_u} \int_{h_u} Q_z(u, v) du$$

$$Q_n(u) = \frac{1}{h_v} \int_{h_v} Q_z(u, v) dv$$

$$\bar{Q} = \frac{1}{h_u h_v} \int_{h_u h_v} Q_z(u, v) dv du$$

Using the same arguments as for the inhomogeneous source, we may neglect the source term contribution from $Q_n(v)$ and $\bar{Q}$. The resulting contribution is expanded into Legendre polynomials as before:

$$\frac{1}{h_u} \int_{h_u} \sum_{l=1}^L g_l P_l(u) Q_z(u, v) du = \sum_{l=1}^L \frac{g_l q_l^u}{2l+1} \quad (3.38)$$

with

$$q_l^u = \frac{2l+1}{h_u} \int_{h_u} Q_n(u) P_l\left(\frac{2u}{h_u}\right) du$$

The source term $Q_n(v)$ given in eq. (3.34) may then be expressed as:

$$Q_n(v) = \frac{q_n(v)}{K} + \sum_{l=1}^L \frac{g_l q_l^u}{2l+1} \quad (3.39)$$

This expression contains some interesting characteristics. The source term in the v -direction is given as two components. The first as the standard one-dimensional source $q_n(v)$ scaled by the mapped node size ratio K , and the second as a contribution of higher order source moments from the radial direction. The mapped azimuthal source term carries a radial contribution.

Factored variable separation - inhomogeneous geometric source

On the other hand, if we assume the following approximation for the two-dimensional flux:

$$\Phi_z(u, v) = \frac{f_n(u) f_n(v)}{\bar{f}} \quad (3.40)$$

and substitute it into eq. (3.33), we find:

$$s_n(v) = -\sigma_n^{\text{rem}} \frac{1}{h_u} \frac{f_n(v)}{\bar{f}} \int_{h_u} \sum_{l=1}^L g_l P_l\left(\frac{2u}{h_u}\right) f_n(u) du$$

Furthermore, we expanding both the u and v one-dimensional flux in Legendre polynomials:

$$\begin{aligned} s_n(v) &= -\sigma_n^{\text{rem}} \frac{\sum_{l=0}^L f_l^v P_l\left(\frac{2v}{h_v}\right)}{\bar{f}} \sum_{l=1}^L \frac{g_l f_l^u}{2l+1} \\ s_n(v) &= -\sigma_n^{\text{rem}} \sum_{l=1}^L \frac{g_l f_l^u}{2l+1} \left(1 + \frac{\sum_{l=1}^L f_l^v P_l\left(\frac{2v}{h_v}\right)}{\bar{f}} \right) \end{aligned} \quad (3.41)$$

We notice that, using the factored separation, the inhomogeneous source in the v direction maintains some functional dependence on v , with an average value equal to that of the summative separation assumption in the previous section.

Factored variable separation - standard source term

We apply variable separation to the two-dimensional source term in product form and define:

$$Q(u, v) = \frac{q_n(u)q_n(v)}{Q} \quad (3.42)$$

We apply it to eq. (3.34) and write

$$Q_n(v) = \frac{q_n(v)}{K} + \frac{1}{h_u} \int_{h_u} \sum_{l=1}^L g_l P_l(u) Q_n(u, v) du = \frac{q_n(v)}{K} + \frac{q_n(v)}{Q h_u} \int_{h_u} \sum_{l=1}^L g_l P_l(u) Q_n(u) du$$

Utilizing one-dimensional source moments in u and v direction, this equation may be reduced to:

$$\begin{aligned} Q_n(v) &= \frac{q_n(v)}{K} + \frac{q_n(v)}{Q} \sum_{l=1}^L \left(\frac{g_l}{h_u} \int_{h_u} P_l(u) Q_n(u) du \right) = \frac{q_n(v)}{K} + \frac{1}{2l+1} \frac{q_n(v)}{Q} \sum_{l=1}^L g_l q_l^u \\ &= q_n(v) \left(\frac{1}{K} + \frac{\frac{1}{2l+1} \sum_{l=1}^L g_l q_l^u}{q_0^u} \right) \end{aligned} \quad (3.43)$$

Summary term analysis for v -equation

The four alternatives described above, namely the factored or summed approach applied to both the standard and inhomogeneous v -dependent sources, all provide the means of completing the transverse integration over u . For the sake of this work, the slightly simpler summed approach will be applied to both sources, and the impact of the additional higher order terms from the factored variable separation will be left as future work.

To conclude the formulation of the one-dimensional v -equation, a summary of the required expansions is given.

1. $L_{n,v}^z(v)$ and $L_{n,v}^u(v)$ will be expressed in terms of Legendre polynomial as $L_{n,v}(v) =$

$\sum_{l=0}^L l_l^v P_l(\frac{2v}{h_v})$. These expansions are described in Section 3.9.

2. $s_n(v) = -\sigma_n^{rem} \sum_{l=1}^L \frac{g_l f_l^v}{2l+1}$ This expression requires, once again, moments of the mapping function as well as flux moments in the u direction. These expansions are developed in Section 3.5.1.

3. $Q_n(v) = \frac{q_n(v)}{K} + \sum_{l=1}^L \frac{g_l q_l^v}{2l+1}$. Notice here that the source in v direction is dependent upon the higher order source moments in u direction. Since the summative variable approximation is to be initially implemented into the test code, it is only stated in the summary.

Final Form

With all the terms expressed as Legendre polynomials, we may merge the source terms of eq. (3.31):

$$R_{n,v}(v) = \sum_{l=0}^L d_l^v P_l(\frac{2v}{h_v}) \quad (3.44)$$

$$d_l^v = -l_l^v + \frac{q_l^v}{K} \text{ for } l > 0$$

$$d_0^v = -l_0^v + \frac{q_0^v}{K} - \sigma_n^{rem} \left(\sum_1^L \frac{g_l f_l^v}{2l+1} \right) + \left(\sum_{l=1}^L \frac{g_l q_l^v}{2l+1} \right)$$

3.4.3 Transverse integration over (r, θ) - the z -equation

The process to find a one-dimensional equation in the z -direction is much more analogous to that of pure Cartesian geometry transverse integration [11]. We begin with the cylindrical diffusion equation in three dimensions (eq. (3.1)) and transversely integrate and average over r and θ to obtain:

$$\frac{-D}{S_{r\theta}} \int_{S_{r\theta}} \nabla^2 \Phi(r, \theta, z) S - D \frac{d^2}{dz^2} f_n(z) + \sigma^{rem} f_n(z) = Q_n(z) \quad (3.45)$$

with

$$f_n(z) = \frac{1}{S_{r\theta}} \int_{S_{r\theta}} \Phi(r, \theta, z) dS$$

We transfer the first term of eq. (3.45) to the right hand side applying the divergence theorem in order to express transverse leakage in terms of transverse currents (as was done in the u and v directions):

$$-D \frac{d^2}{dz^2} f_n(z) + \sigma^{rem} f_n(z) = Q_n(z) - L_{n,z}(z) \quad (3.46)$$

$$L_{n,z}(z) = \frac{-D}{S_{r\theta}} \int_{S_{r\theta}} \nabla^2 \Phi(r, \theta, z) S = \frac{-D}{S_{r\theta}} \int_c \vec{n} \cdot \nabla \Phi(r, \theta, z) dl$$

$$L_{n,z}(z) = L_{n,z}^r(z) + L_{n,z}^\theta(z)$$

$$L_{n,z}^r(z) = \frac{J_{n,r}(r_n^-, z) + J_{n,r}(r_n^+, z)}{\Delta r_n}$$

$$L_{n,z}^\theta(z) = \frac{J_{n,\theta}(\theta_n^-, z) + J_{n,\theta}(\theta_n^+, z)}{r_{n,mid} \Delta \theta_n}$$

Summary term analysis of z -equation

In order to solve equation (3.46) we need to calculate the following inhomogeneous terms (expressed in terms of Legendre polynomials). The detailed form of the solution is given in Section 3.7.

1. $L_{n,z}^r(z)$ and $L_{n,z}^\theta(z)$ - these are handled in Section 3.9, but will be expressed in terms of Legendre polynomials as $L_{n,z}(z) = \sum_{l=0}^L l_l^z P_l(\frac{2z}{h_z})$.

$$2. Q_n(z) = \sum_{l=0}^L q_l^z P_l(\frac{2z}{h_z}).$$

This gives the right hand side of eq. (3.46) in terms of Legendre polynomials:

$$R_{n,z}(z) = \sum_{l=0}^L d_l^z P_l(\frac{2z}{h_z}) \quad (3.47)$$

where

$$d_l^z = q_l^z - l_l^z$$

3.4.4 Summary

One-dimensional, auxiliary diffusion equations have now been developed in all three directions (Sections 3.4.1, 3.4.2 and 3.4.3), with the respective source terms in each direction expanded upon a Legendre polynomial base. These equations are in the form of ordinary, linear, inhomogeneous differential equations, and may be solved analytically. The following section will address the issue of developing a one-dimensional solution to each of these equations, and to use it to obtain the elusive node-averaged flux to side-averaged current relationships required to close the system of nodal balance equations (eq. 3.2).

3.5 Solution to the one-dimensional u -equation

The conformal mapping technique, as applied to the diffusion equation in cylindrical geometry, allows us to solve the diffusion problem via the Analytic Nodal Method (ANM) in Cartesian geometry [11]. In the following sections, this fact is exploited, since we now complete the solution of the one-dimensional equations in mapped Cartesian geometry. The only price to pay for the coordinate mapping manifests in the form of the additional inhomogeneous sources, as well as the additional mapping function and scaling factors introduced in Section 3.3.

We may rewrite eq. (3.29) in terms of a normalized variable $w = \frac{2u}{h_n}$. This step is useful, since it transforms the node onto a local coordinate ranging from $[-1, 1]$, and simplifies some of the algebraic expressions to follow. The transversely integrated one-dimensional diffusion equation in w then takes the form:

$$\frac{d^2}{dw^2} f_n(w) + (\beta_n^{nm})^2 f_n(w) = \frac{1}{-D_n} \left(\frac{\eta_n h_{n,w}}{2} \right)^2 R_n(w) \quad (3.48)$$

where

$$R_n(w) = \sum_{l=0}^L d_l P_l(w)$$

Here L is defined as the order of the source term expansion. In eq. (3.48) the moments of the one-dimensional source, d_l , are as yet unknown. They will be developed shortly. If we assume for the moment that they are known, the analytic solution of eq. (3.48) for node n may then be written in the form:

$$f_n(w) = C_1 \cosh(\beta_n^{nm} w) + C_2 \sinh(\beta_n^{nm} w) + \sum_{k=0}^L b_k P_k(w) \quad (3.49)$$

We define

b_k as the moments of the particular solution

$$\begin{aligned} C_1 &= \frac{(f^+ - Z^+) + (f^- - Z^-)}{2\cosh(\beta_n^{nm})} \\ C_2 &= \frac{(f^+ - Z^+) - (f^- - Z^-)}{2\sinh(\beta_n^{nm})} \\ (\beta_n^{nm})^2 &= \left[\frac{\sigma_n^{rem} \left(\frac{r_n h_{n,u}}{2} \right)^2}{-D_n} \right] \end{aligned} \quad (3.50)$$

where once more (as described in Section 3.3)

$$\eta^2 = r_i r_{i+1} \quad (3.51)$$

$$h_{n,u} = \ln(r_{i+1}) - \ln(r_i)$$

$$= \ln \left(\frac{r_{i+1}}{r_i} \right)$$

f^+, f^-, Z^+ and Z^- represents the side values of the flux and the particular solution.

Note here that β_n^{nm} refers to the one-group buckling term for node n , and r_i and r_{i+1} refer to the original inner and outer radial coordinates of radial zone n , respectively. Some clarification is needed here, since the compound superscript index mn , coupled with subscript n , refers to the value of the variable for node n in the direction mn where node m is the neighbour in the current direction of investigation - in this case direction u . Denote further:

$$\overline{\beta_n^{nm}} = \text{Imag}(\beta_n^{nm}) = \sqrt{|(\beta_n^{nm})^2|} \quad (3.52)$$

It is possible, by utilizing the orthogonality properties of Legendre polynomials, to express the moments of the particular solution directly in terms of the source moments. The particular solution may be obtained directly from the source term by the following recursive relationship:

$$b_L = \frac{1}{(\beta_n^{mn})^2} \left(\frac{\eta h_{n,u}}{2} \right)^2 D_n^{-1} d_L = -\frac{1}{\sigma_n^{rem}} d_L, \quad (3.53)$$

$$b_{L-1} = \frac{1}{(\beta_n^{mn})^2} \left(\frac{\eta h_{n,u}}{2} \right)^2 D_n^{-1} d_{L-1} = -\frac{1}{\sigma_n^{rem}} d_{L-1}, \quad (3.54)$$

$$b_l = \frac{1}{(\beta_n^{mn})^2} \left[\left(\frac{\eta h_{n,u}}{2} \right)^2 D_n^{-1} d_l - \sum_{m=l+2}^L a_{lm} b_m \right], \quad l = L-2, \dots, 1, 0 \quad (3.55)$$

with

$$a_{lm} = \frac{2l+1}{4} [1 + (-1)^{l+m}] [m(m+1) - l(l+1)] \quad (3.56)$$

These b_l coefficients are used in obtaining the expressions for Z^+ and Z^- in eq. (3.49).

$$Z^+ = \sum_{k=0}^L b_k$$

$$Z^- = \sum_{k=0}^L b_k (-1)^k$$

We also denote the side fluxes as node interface fluxes

$$f^+ = \phi_{n,n+1}^{mn}$$

$$f^- = \phi_{n-1,n}^{mn}$$

Here $\phi_{n-1,n}^{mn}$ refers to the side flux in direction mn on the surface between nodes $n-1$ and n .

Determination of source moments

The remaining issue in completing the solution in the u -direction is constructing the Legendre expansion moments for the source term in the radial direction. The source is constructed in mapped u coordinates in eq. (3.57), and represents the summation of the regular (fission and scattering), inhomogeneous and transverse leakage sources:

$$R_{n,u}(u) = g(u)^2 Q_n(u) + S_n(u) - L_{n,u}(u) = \sum_{l=0}^L d_l^u P_l\left(\frac{2u}{h_u}\right) \quad (3.57)$$

with

$$\begin{aligned}
L_{n,u}(u) &= \sum_{l=0}^L l_l^u P_l\left(\frac{2u}{h_u}\right) \\
S_n(u) &= (1 - g(u)^2) \sigma_n^{rem} f_n(u) = \sum_{l=0}^L s_l^u P_l\left(\frac{2u}{h_u}\right) \\
s_l^u &= \frac{2l+1}{h_u} \int_{h_u} (1 - e^{2u}) \sigma_n^{rem} f_n(u) P_l\left(\frac{2u}{h_u}\right) du \\
g(u)^2 Q_n(u) &= \sum_{l=0}^L q_l^u P_l\left(\frac{2u}{h_u}\right) \\
q_l^u &= \frac{2l+1}{h_u} \int_{h_u} e^{2u} Q_n(u) P_l\left(\frac{2u}{h_u}\right) du
\end{aligned}$$

We rewrite these expressions in terms of normalized w coordinates to yield

$$R_{n,u}(w) = g(w)^2 Q_n(w) + S_n(w) - L_{n,u}(w) = \sum_{l=0}^L d_l P_l(w) \quad (3.58)$$

with transverse leakage

$$L_{n,u}(w) = \sum_{l=0}^L l_l^u P_l(w)$$

and inhomogeneous source

$$\begin{aligned}
S_n(w) &= (1 - g(w)^2) \sigma_n^{rem} f_n(w) = \sum_{l=0}^L s_l^u P_l(w) \\
s_l^u &= \frac{2l+1}{2} \int_{-1}^1 (1 - e^{wh_u}) \sigma_n^{rem} f_n(w) P_l(w) dw \\
&= \frac{\sigma_n^{rem}(2l+1)}{2} \left(\int_{-1}^1 f_n(w) P_l(w) dw - \int_{-1}^1 e^{wh_u} f_n(w) P_l(w) dw \right)
\end{aligned}$$

and the regular nodal source

$$\begin{aligned}
g(w)^2 Q_n(w) &= \sum_{l=0}^L q_l^u P_l(w) \\
Q_n(w) &= Q_n^{fission}(w) + Q_n^{scatter}(w) + Q_n^{fixed}
\end{aligned}$$

$$Q_n^{fission}(w) = \frac{1}{k_{eff}} \chi^g \sum_{h=1}^G v \sigma_{f,n}^h f^h(w)$$

$$Q_n^{scatter}(w) = \sum_{h=1, h \neq g}^G \sigma_{s0,n}^{h-g} f^h(w)$$

$$q_l^u = \frac{(2l+1)}{2} \int_{-1}^1 Q(w)_n e^{h_u w} P_l(w) dw$$

$$q_l^u = q_l^{fission} + q_l^{scatter} + q_l^{fixed}$$

Once these moments are calculated:

$$d_l = -l_l^u + q_l^u + s_l^u \quad (3.59)$$

Some investigation of the definition of the required moments, will show that some support quantities, to be termed **flux moments** and **mapped flux moments**, occur often and can be independently calculated. These flux moments are used to construct the required source moments, i.e. fission source, scattering source and inhomogeneous source. These expansions are developed in the next section largely as recurrence relationships to facilitate variable expansion order calculations.

3.5.1 Calculation of moments

A significant component of this work is the efficient representation of non-linear sources in the one-dimensional equations, and as such, the calculation for higher order expressions for the one-dimensional flux. These expressions are developed in this section, so far possible to arbitrary polynomial order.

Flux Moments

The flux moments are calculated via recurrence relationships and some explicit integrals. Expressions for the one-dimensional flux moments will allow the calculation of some of the components of d_l in exp. (3.59). We will proceed in order to find Legendre expansion coefficients for the expression:

$$f_n(w) = \sum_{l=0}^L f_l^n P_l(w) \quad (3.60)$$

and term the coefficients f_l^u **flux moments**. Using the analytic solution (3.49), we have

$$f_l^u = \frac{2l+1}{2}(C_1 f_l^{\cos} + C_2 f_l^{\sin}) + b_l \quad (3.61)$$

where we define the hyperbolic cosine moments

$$f_l^{\cos} = \int_{-1}^1 \cosh(\beta w) P_l(w) dw \quad (3.62)$$

and hyperbolic sine moments

$$f_l^{\sin} = \int_{-1}^1 \sinh(\beta w) P_l(w) dw \quad (3.63)$$

These moments are calculated via derived recurrence relations and are given in Appendix E.

Mapped Flux moments

We also come across expressions of the following form, and term the moments of this expression **mapped flux moments**:

$$g^2(w) f_n(w) = \sum_{l=0}^L (fg)_l^u P_l(w) \quad (3.64)$$

Using analytic solution (3.49), we have

$$(fg)_l^u = \frac{2l+1}{2}(C_1 (fg)_l^{\cos} + C_2 (fg)_l^{\sin}) + (fg)_l^Z \quad (3.65)$$

where we defined the mapped hyperbolic cosine moments

$$(fg)_l^{\cos} = \int_{-1}^1 \cosh(\beta w) e^{h_w w} P_l(w) dw$$

and the mapped hyperbolic sine moments

$$(fg)_l^{\sin} = \int_{-1}^1 \sinh(\beta w) e^{h_w w} P_l(w) dw$$

These mapped moments are calculated via recurrence relationships derived in Appendix E. There are however difficulties in deriving a recurrence relationship for the particular solution part of the one-dimensional flux, as this term forms a double Legendre - exponential integral:

$$(fg)_i^Z = \sum_{k=0}^L b_k \int_{-1}^1 e^{h_u w} P_k(w) P_i(w) dw$$

These integrals are calculated explicitly (15 in total since they are symmetric fourth order integrals) with the support of the software package Mathematica [4]. The expressions for these integrals, in the form of both their analytic and Taylor series forms (required to eliminate potential round-off errors), are given in Appendix F.

Moments of the mapping function

Finally we need to define an expression for moments of the mapping function.

$$g^2(u) = e^{2u} = e^{h_u w} = g^2(w) = \sum_{l=0}^L g_l^u P_l(w) \quad (3.66)$$

with

$$g_l^u = \frac{(2l+1)}{2} \int_{-1}^1 e^{h_u w} P_l(w) dw$$

Using recurrence relation (E.1) we express:

$$g_l^u = \frac{(2l+1)}{2} \left(-\frac{2l-1}{h_u} I_{l-1} + I_{l-2} \right) \quad (3.67)$$

$$I_0 = \frac{2}{h_u} \sinh(h_u), \quad I_1 = \frac{2}{h_u} \left(\cosh(h_u) - \frac{\sinh(h_u)}{h_u} \right)$$

$$I_l = -\frac{2l-1}{h_u} I_{l-1} + I_{l-2}$$

$$g_0^u = \frac{I_0}{2}$$

$$g_1^u = \frac{3I_1}{2}$$

Final form of source moments

The constructions in the previous section allow us to describe, in a clear form, all sources within the one-dimensional u -equation. These expressions, now developed up to an arbitrary order, are presented in this section.

Scattering source moments

$$q_l^{\text{scatter}} = \sum_{h=1, h \neq g}^G \sigma_{s0,n}^{h \rightarrow g} ((fg)_l^h) \quad (3.68)$$

Fission source moments

$$q_l^{\text{fission}} = \frac{1}{k_{eff}} \chi^g v^g \sum_{h=1}^G \sigma_{f,u}^h ((fg)_l^h) \quad (3.69)$$

Inhomogeneous Source moment expression

We may now put eqs. (3.61) and (3.65) together to yield the following expression for the inhomogeneous source moments in the mapped u direction:

$$\begin{aligned} s_l^u &= \frac{\sigma_n^{\text{rem}}(2l+1)}{2} \left(\int_{-1}^1 f_n(w) P_l(w) dw - \int_{-1}^1 e^{wh_u} f_n(w) P_l(w) dw \right) \\ &= \sigma_n^{\text{rem}} (f_l^u - (fg)_l^u) \end{aligned} \quad (3.70)$$

Fixed source moment expression

The moments for the fixed source term may be expressed in terms of the mapping function moments defined in eq. (3.67):

$$\begin{aligned} q_l^u &= \frac{(2l+1)Q_n^{\text{fixed}}}{2} \int_{-1}^1 e^{h_u w} P_l(w) dw \\ &= Q_n^{\text{fixed}} g_l^u \end{aligned}$$

Transverse leakage moment expression

The transverse leakage moments are defined across multiple nodes, and their treatment is left for Section 3.9 when all three one-dimensional equation solutions have been appropriately formulated.

3.5.2 Current and flux expressions

From the one-dimensional solution (3.49), we can derive the expression for both the surface-averaged current, as well as the expression for side-averaged fluxes. These solutions are

derived from a constructed two-node problem, and are consistent with the formalism of the standard ANM as implemented in the Necsa based MGRAC code [22]. We obtain

$$\bar{J}_{mn} = d_n^{mn} s_n^{mn} [\bar{f}_n - Z_{mn}] - d_n^{mn} \phi_{n,m}^{mn} \quad (3.71)$$

$$\phi_{n,m}^{mn} = s_n^{mn} [\bar{f}_n - Z_{mn}] - \frac{\bar{J}_{mn}}{d_n^{mn}} \quad (3.72)$$

where we have defined the “tensorial source” as:

$$\begin{aligned} Z_{mn} &= \frac{1}{-D_n} \frac{(\frac{\eta h_w}{2})^2}{2(\beta_n^{nm})^2} \int_{-1}^1 (1 - \cosh(\beta_n^{nm} \pm \beta_n^{nm} w)) R_n(w) dw \\ &= \frac{1}{2\sigma_n^{rem}} \int_{-1}^1 (1 - \cosh(\beta_n^{nm} \pm \beta_n^{nm} w)) R_n(w) dw \end{aligned} \quad (3.73)$$

and

$$\begin{aligned} t_n^{mn} &= \frac{\overline{\beta_n^{nm}}}{\tanh(\beta_n^{nm})} \\ d_n^{mn} &= (\frac{2}{h_{w,n}}) D_n t_n^{mn} \\ s_n^{mn} &= \frac{2\overline{\beta_n^{nm}}}{\sinh(2\beta_n^{nm})} \end{aligned}$$

Using equation (3.49) over two neighbouring nodes, and applying flux and current continuity conditions at the interface, expressions for the one-dimensional side-averaged current may be obtained in terms of the node-averaged quantities.

$$\bar{J}_{mn} = d_{mn} s_n^{mn} [\bar{f}_n - Z_{mn}] - d_{mn} s_m^{mn} [\bar{f}_m - Z_{nm}]$$

where

$$d_{mn} = [(d_n^{mn})^{-1} + (d_m^{mn})^{-1}]^{-1}$$

The side fluxes calculated in eq. (3.72) are necessary in order to define the constants C_1 and C_2 of the one-dimensional solution. An important difference from the standard ANM is that the currents obtained in this formulation are defined as currents within the mapped u direction, and have to be redefined per eq. (3.27) prior to inserting them into the

balance relation (3.2). We therefore present expression (3.74) as an important result from this section:

$$\bar{J}_{mn} = C_{mn}^r (\bar{f}_n - Z_{mn}) - C_{nm}^r (\bar{f}_m - Z_{nm}) \quad (3.74)$$

with

$$C_{mn}^r = \frac{1}{r_{mn}} d_{nm} s_n^{mn}$$

$$C_{nm}^r = \frac{1}{r_{mn}} d_{nm} s_m^{mn}$$

where r_{mn} is the radial boundary between mesh m and mesh n . Stating for clarity the relationship between mapped and unmapped currents:

$$\bar{J}_{n-1,n} = \frac{1}{r_{n-1,n}} \frac{2}{h_{w,n}} \bar{J}_{n-1,n} \quad (3.75)$$

Only two issues remain before reinserting eq. (3.74) into the balance equation (3.2), having then obtained the necessary information from the auxiliary one-dimensional u equation.

- The quantity defined as the “tensorial source” must be expressed in terms of calculated moments. We use the term “tensorial” because this source has different values at the left and the right surfaces of the node.
- The earlier defined relationship between the original coordinate system node-averaged flux and one-dimensional average flux (eq. 3.26) must be used to adjust eq. (3.74) in such a way that the side-averaged current is expressed in terms of the node-averaged flux instead of one-dimensional average. This will be done by redefining the tensorial source quantity.

Both the above two points are addressed in the following section in which the tensorial source is described.

3.5.3 Tensorial source

Having obtained all moments related to the Legendre expansion for the source term in eq. (3.73), we may proceed to calculate the tensorial source Z_{mn} . The tensorial source is used in the calculation of surface-averaged net currents, and carries the source terms from iteration to iteration (along with the moments of the particular solution used to calculate the one-dimensional solution constants). We express

$$Z_{mn} = \frac{(\frac{\eta h_u}{2})^2}{-2(\beta_n^{nm})^2 D_n} \int_{-1}^1 ((1 - \cosh(\beta_n^{nm} \pm \beta_n^{nm} w)) R_n(w) dw \quad (3.76)$$

$$\int_{-1}^1 ((1 - \cosh(\beta_n^{nm} + \beta_n^{nm} w)) R_n(w) dw = d_0 - \frac{1}{2} \sum_{l=0}^L d_l [\cosh(\beta_n^{nm}) f_l^{\cos} + \sinh(\beta_n^{nm}) f_l^{\sin}]$$

$$\int_{-1}^1 ((1 - \cosh(\beta_n^{nm} - \beta_n^{nm} w)) R_n(w) dw = d_0 - \frac{1}{2} \sum_{l=0}^L d_l [\cosh(\beta_n^{nm}) f_l^{\cos} - \sinh(\beta_n^{nm}) f_l^{\sin}]$$

Here $f_l^{\cos}$ and $f_l^{\sin}$ refer to the quantities defined in eqs. (3.62) and (3.63) respectively. After some simplification, expressions for the tensorial source may be written as:

$$Z_{mn}^{right} = \frac{(\frac{\eta h_u}{2})^2}{-D_n(\beta_n^{nm})^2} \left(d_0 - \frac{1}{2} \sum_{l=0}^L d_l [\cosh(\beta_n^{nm}) f_l^{\cos} + \sinh(\beta_n^{nm}) f_l^{\sin}] \right) \quad (3.77)$$

$$Z_{mn}^{left} = \frac{(\frac{\eta h_u}{2})^2}{-D_n(\beta_n^{nm})^2} \left(d_0 - \frac{1}{2} \sum_{l=0}^L d_l [\cosh(\beta_n^{nm}) f_l^{\cos} - \sinh(\beta_n^{nm}) f_l^{\sin}] \right) \quad (3.78)$$

Mapping impact on tensorial definition

The coordinate transformation implies a certain relationship between node-averaged flux and one-dimensional averages in the u and v direction. This relationship was developed and presented in eq. (3.26). Within a purely Cartesian framework, one-dimensional average fluxes are equal to node-averaged flux, and obviates this discussion. In our case, due to the u -dependent mapping function, and the separation of variable approximation, a distinct relationship between one-dimensional u and v -averages and node-averaged fluxes, exist. The separation of variable approximation, and the definition of node-averaged flux are once more stated below:

$$\Phi_n(u, v) = f_n(u) + f_n(v) - \bar{f} \quad (3.79)$$

$$\bar{\Phi}_n = \frac{1}{h_u h_v} \int_{h_u} \int_{h_v} \Phi_n(u, v) g(u)^2 du dv \quad (3.80)$$

remembering that the area element $r dr d\theta$ was mapped onto $g(u)^2 du dv$ during conformal mapping. Furthermore,

$$\bar{f} = \bar{f}_u = \bar{f}_v \quad (3.81)$$

since

$$f_n(u) = \int_{h_v} \Phi_n(u, v) dv \quad (3.82)$$

and

$$f_n(v) = \int_{h_u} \Phi_n(u, v) du \quad (3.83)$$

It is important to then apply the relationship between $\bar{f}$ and $\bar{\Phi}_n$, since the side-averaged current to node-averaged flux relationship can only be found if it is known. As stated in eq. (3.74), we have:

$$\bar{J}_{mn} = C_{mn}^r(\bar{f}_n - Z_{mn}) - C_{nm}^r(\bar{f}_m - Z_{nm}) \quad (3.84)$$

We need to (after solving a two node problem to obtain this relationship) express this relationship in terms of node-averaged flux, and not purely in terms of one-dimensional average. We therefore need:

$$\bar{J}_{mn} = C_{mn}^r(\bar{\Phi}_n - \delta Z_{mn}) - C_{nm}^r(\bar{\Phi}_m - \delta Z_{nm}) \quad (3.85)$$

We can, due to (3.81), only consider the relationship between one-dimensional average in u and node-averaged flux (will be the same in v -direction). The obtained node-averaged flux to one-dimensional average in u is (restated here for easy reference):

$$\bar{\Phi}_n = \bar{f}_n + K \sum_{l=1}^{\infty} \frac{f_l^u g_l}{2l+1} \quad (3.86)$$

Redefinition of tensorial source

Using eq. (3.86) we may, as an initial suggestion, redefine the tensorial quantity as follows:

$$\delta Z_{mn}^{right, left} = Z_{mn}^{right, left} + K \sum_{l=1}^{\infty} \frac{f_l^u g_l}{2l+1} \quad (3.87)$$

and remain with

$$\bar{J}_{mn} = C_{mn}^r(\bar{\Phi}_n - \delta Z_{mn}) - C_{nm}^r(\bar{\Phi}_m - \delta Z_{nm}) \quad (3.88)$$

This approach will do and we have obtained the all important side-averaged current to node-averaged current relationship. Nevertheless, exp. (3.88) may yield initial numerical

instabilities, since eq. (3.81) is only guaranteed to be valid upon system convergence. It would be preferable to include the node-averaged flux in the definition of tensorial in a slightly more elegant fashion. The following approach is presented here purely as an alternative when and if such convergence problems arise.

Consider the contribution of the u -direction inhomogeneous source to the tensorial quantity (define the remaining source contribution as Z_{mn}^{rem} i.e. $Z_{mn} = Z_{mn}^{rem} + Z_{mn}^{inh}$):

$$Z_{mn}^{inh} = \frac{1}{2} \int_{-1}^1 (1 - \cosh(\beta_n^{nm} \pm \beta_n^{nm} w)) (f(w) - f(w)g(w)^2) dw \quad (3.89)$$

$$Z_{mn}^{inh} = \frac{1}{2} \int_{-1}^1 (f(w) - f(w)g(w)^2) dw + \left(-\frac{1}{2} \int_{-1}^1 \cosh(\beta_n^{nm} \pm \beta_n^{nm} w) (f(w) - f(w)g(w)^2) dw \right) \quad (3.90)$$

We may identify the first of these integrals as possessing two components:

$$Z_{mn}^{inh,1} = \frac{1}{2} \int_{-1}^1 (f(w) - f(w)g(w)^2) dw = \bar{f}_n - \bar{\Phi}_n$$

$$Z_{mn}^{inh,1} = \bar{f}_n - \bar{\Phi}_n$$

defining the remaining integral as:

$$Z_{mn}^{inh,2,left:right} = -\frac{1}{2} \int_{-1}^1 \cosh(\beta_n^{nm} \pm \beta_n^{nm} w) (f(w) - f(w)g(w)^2) dw$$

Replacing this definition within eq. (3.84), yields:

$$\bar{J}_{mn}^r = C_{mn}^r (\bar{\Phi}_n - (Z_{mn}^{inh,2} + Z_{mn}^{rem})) - C_{nm}^r (\bar{\Phi}_m - (Z_{mn}^{inh,2} + Z_{mn}^{rem})) \quad (3.91)$$

The remaining component of the inhomogeneous source needs to be calculated, and revolves around the quantity:

$$Z_{mn}^{inh,2} = -\frac{1}{2} \int_{-1}^1 \cosh(\beta_n^{nm} \pm \beta_n^{nm} w) (f(w) - f(w)g(w)^2) dw \quad (3.92)$$

which may be written in terms of previously defined moments as:

$$Z_{mn}^{inh,2} = -\frac{1}{2\sigma_{rem}} \sum_{l=0}^L s_l^u [\cosh(\beta_n^{nm}) f_l^{cos} + \sinh(\beta_n^{nm}) f_l^{sin}] \quad (3.93)$$

Definition (3.91) allows the definition of side-averaged currents in terms of node-averaged

fluxes by limiting the contribution of the inhomogeneous source to the tensorial, and further limits the numerical dependence of the test code on calculated flux moments, which in turn depends, in the initial stages of calculation, on potential disruptive initial guesses. Although this method is more elegant, the structure of the test code is such that the appropriate relationship between one-dimensional average and node-averaged flux is maintained during all iteration levels. For this reason the approach as described in eq. (3.87) is implemented.

3.6 Solution to the one-dimensional v -equation

The same analysis and development that had been performed in the previous section to formulate a node-averaged flux to side-averaged current relationship is now repeated for the v -direction. The process is briefly restated, and issues particular to the solution in the v -direction are highlighted. The transversely integrated one-dimensional diffusion equation in v is given as

$$\frac{d^2}{dw^2} f_n(w) + (\beta_n^{nm})^2 f_n(w) = \frac{1}{-D_n} \left(\frac{\eta_n h_{n,w}}{2} \right)^2 R_n(w) \quad (3.94)$$

$$R_n(w) = \sum_{l=0}^L d_l P_l(w) = Q_n(v) + s_n(v) - L_{n,v}(v)$$

$$s_n(v) = \sigma_n^{rem}(\bar{f}) - \frac{1}{h_u} \int_{h_u} g(u)^2 f_n(u) du$$

$$Q_n(v) = \frac{q_n(v)}{K} + \frac{1}{h_u} \int_{h_u} \sum_{l=1}^L g_l P_l\left(\frac{2u}{h_u}\right) Q_z(u, v) du$$

The analytical solution of equation (3.94) with $w = \frac{2v}{h_v}$ for node n may be written in the form:

$$f_n(w) = C_{n,1} \cosh(\beta_n^{nm} w) + C_{n,2} \sinh(\beta_n^{nm} w) + \sum_{k=0}^L b_k P_k(w) \quad (3.95)$$

where we define

$$C_1 = \frac{(f^+ - Z^+) + (f^- - Z^-)}{2 \cosh(\beta_n^{nm})}$$

$$C_2 = \frac{(f^+ - Z^+) - (f^- - Z^-)}{2 \sinh(\beta_n^{nm})}$$

$$(\beta_n^{nm})^2 = \left[\frac{\sigma_n^{+em} \left(\frac{\eta_n h_{n,u}}{2} \right)^2}{-D_n K} \right] \quad (3.96)$$

with

$$\eta^2 = r_n r_{n+1} \quad (3.97)$$

$$h_{n,v} = \Delta \theta_n$$

and let further:

$$\overline{\beta_n^{nm}} = \text{Imag}(\beta_n^{nm}) = \sqrt{|(\beta_n^{nm})^2|} \quad (3.98)$$

The particular solution is obtained directly from the source term by the following recursive relationship:

$$b_L = \frac{1}{(\beta_n^{nm})^2} \left(\frac{\eta h_w}{2} \right)^2 D_n^{-1} d_L, \quad (3.99)$$

$$b_{L-1} = \frac{1}{(\beta_n^{nm})^2} \left(\frac{\eta h_w}{2} \right)^2 D_n^{-1} d_{L-1}, \quad (3.100)$$

$$b_l = \frac{1}{(\beta_n^{nm})^2} \left[\left(\frac{\eta h_w}{2} \right)^2 D_n^{-1} d_l - \sum_{m=l+2}^L a_{lm} b_m \right], \quad l = L-2, \dots, 1, 0 \quad (3.101)$$

with

$$a_{lm} = \frac{2l+1}{4} [1 + (-1)^{l+m}] [m(m+1) - l(l+1)] \quad (3.102)$$

These b_l coefficients are used in obtaining the expressions for C_1 and C_2 in eqs. (3.103) and (3.104).

$$C_1 = \frac{(f^+ - Z^+) + (f^- - Z^-)}{2 \cosh(\overline{\beta_n^{nm}})} \quad (3.103)$$

$$C_2 = \frac{(f^+ - Z^+) - (f^- - Z^-)}{2 \sinh(\overline{\beta_n^{nm}})} \quad (3.104)$$

$$Z^+ = \sum_{k=0}^L b_k$$

$$Z^- = \sum_{k=0}^L b_k (-1)^k$$

$$f^+ = \phi_{n,n+1}^{min}$$

$$f^- = \phi_{n,n-1}^{min}$$

3.6.1 Determination of source moments

The issue once again is constructing the Legendre expansion moments for the source term in the azimuthal direction. The source is constructed from the following terms, here defined in mapped v -coordinates. The expressions for $s_n(v)$ and $Q_n(v)$ have been expanded and simplified as described in Section 3.4.2.

$$R_n(v) = \sum_{l=0}^L d_l P_l\left(\frac{2v}{h_v}\right) = Q_n(v) + s_n(v) - L_{n,v}(v) \quad (3.105)$$

$$s_n(v) = -\sigma_n^{rem} \frac{1}{h_u} \int_{h_u} \sum_{l=1}^L g_l P_l\left(\frac{2u}{h_u}\right) \Phi_z(u, v) du$$

$$Q_n(v) = \frac{q_n(v)}{K} + \frac{1}{h_u} \int_{h_u} \sum_{l=1}^L g_l P_l\left(\frac{2u}{h_u}\right) Q_z(u, v) du$$

$$L_{n,v}(v) = \sum_{l=0}^L l_l^v P_l\left(\frac{2v}{h_v}\right)$$

We may rewrite these expressions for the normalized dimensionless coordinate $w = \frac{2v}{h_v}$, and denote the normalized u direction dimensionless variable with $u_n = \frac{2u}{h_u}$:

$$R_n(w) = \sum_{l=0}^L d_l P_l(w) = Q_n(w) + s_n(w) - L_{n,v}(w) \quad (3.106)$$

$$s_n(w) = \frac{-\sigma_n^{rem}}{h_u} \int_{-1}^1 \sum_{l=1}^L g_l P_l(u_n) f_n(u_n) du_n = s_0$$

$$Q_n(w) = \frac{q_n(w)}{K_n} + \frac{1}{h_u} \int_{-1}^1 \sum_{l=1}^L g_l P_l(u_n) \sum_{l'=0}^L q_{l'} P_{l'}(u_n) du_n$$

$$q_n(w) = \sum_{l=0}^L q_l^w P_l(w)$$

$$q_n(w) = q_n^{fission}(w) + q_n^{scatter}(w) + q_n^{fixed}$$

$$Q_n^{fission}(w) = \frac{1}{k_{eff}} \chi^g \sum_{h=1}^G v \sigma_{f,n}^h f^h(w)$$

$$Q_n^{scatter}(w) = \sum_{h=1, h \neq g}^G \sigma_{s0,n}^{h \rightarrow g} f^h(w)$$

$$L_n(w) = \sum_{l=0}^L l_l^w P_l(w)$$

$$d_0 = s_0 - l_0^w + \frac{q_0^v}{K} + \sum_{l=1}^L \frac{g_l q_l^u}{2l+1} \quad (3.107)$$

$$d_l = -l_l^w + q_l^v, l \geq 1$$

The source term in the v -direction contains contributions from higher order terms in the u -direction. Even though this contribution appeared due to the application of variable separation, it is consistent with the central issue in cylindrical geometry that the solution in the θ -equation is dependent upon r . This derivation was given in Section 3.4.2.

Calculation of moments

In the v -direction only moments of the one-dimensional flux are required, and only for use in the fission and scattering sources (the inhomogeneous source in the v -direction is constant in v). The definition and recurrence relations required are analogous to the development in the u -direction in Section 3.5.1, and will not be rederived here. Flux moments are expressed as:

$$f_l^v = \frac{2l+1}{2} (C_1 f_l^{v,\cos} + C_2 f_l^{v,\sin}) + b_l \quad (3.108)$$

with $f_l^{v,\cos}$ and $f_l^{v,\sin}$ recursively calculated as in Section 3.5.1.

Final form of source moments

For the sake of easy reference, the various source terms relevant to the solution in the v -direction are listed in this section.

Inhomogeneous source moment expression

The expression for s_0 , which is constant in w , is calculated using eq. (3.109). This expression uses the summative variable separation technique as discussed in Section 3.4.2. We refer to eq. (3.36) and restate

$$s_0^v = -\sigma_n^{rem} \sum_{l=1}^L \frac{g_l f_l^u}{2l+1} \quad (3.109)$$

with

$$g_l = \frac{2l+1}{2} \int_{h_u} e^{h_u u_n} P_l(u_n) du$$

and

$$f_l^u = \frac{2l'+1}{2} \int_{h_u} f_n(u_n) P_{l'}(u_n) du$$

Note that f_l^u and g_l are calculated from Section 3.5.1.

Scattering source moments

$$q_i^{scatter} = \sum_{h=1, h \neq g}^G \sigma_{s0,n}^{h \rightarrow g} ((f)_i^h) \quad (3.110)$$

Fission source moments

$$q_i^{fission} = \frac{1}{k_{eff}} \chi^g \sum_{h=1}^G v^g \sigma_{f,n}^h ((f)_i^h) \quad (3.111)$$

Fixed source moment expression

The moments for the fixed source term may be expressed as:

$$q_0^v = \frac{Q_n^{fixed}}{K} \quad (3.112)$$

Transverse leakage moment expression

The transverse leakage moments are defined across multiple nodes, and their treatment is left for Section 3.9 when all three one-dimensional equation solutions have been appropriately formulated.

Total source moment in v -direction

The total v -dependent source, including the contribution from the u -direction, is given by:

$$Q_n(w) = \frac{q_n(w)}{K} + \sum_{l=1}^L \frac{g_l q_l^u}{2l+1} \quad (3.113)$$

In the case of fission and scattering sources, a series of higher order terms from the u -direction will contribute to the source term in the v -direction.

3.6.2 Current and flux expressions

Once again, analogous to the development in the u -direction, but this time in the v -direction, the expressions for side-averaged current and side-averaged flux are presented:

$$\bar{J}_{mn} = d_n^{mn} s_n^{mn} [\bar{\Phi}_n - Z_{nm}] - d_n^{mn} \phi_{n,m}^{mn} \quad (3.114)$$

$$\phi_{n,m}^{mn} = s_n^{mn} [\bar{\Phi}_n - Z_{nm}] - \frac{\bar{J}_{mn}}{d_n^{mn}} \quad (3.115)$$

with

$$Z_{mn} = \frac{1}{2\sigma_n^{rem}} \int_{-1}^1 (1 - \cosh(\beta_n^{mn} \pm \beta_n^{mn} w)) R_n(w) dw \quad (3.116)$$

$$t_n^{mn} = \frac{\overline{\beta_n^{mn}}}{\tanh(\overline{\beta_n^{mn}})}$$

$$d_n^{mn} = \left(\frac{2}{h_w}\right) D_n t_n^{mn}$$

$$s_n^{mn} = \frac{2\overline{\beta_n^{mn}}}{\sinh(2\overline{\beta_n^{mn}})}$$

These expressions culminate into a surface-averaged current to node-averaged flux relationship, taking care to scale them appropriately to yield the side-averaged current in original coordinates (utilizing definitions from Section 3.3.1). Once more (as was the case in

the u -direction) we obtain an important result in this section as we define the net current expressions in the v -direction:

$$\bar{J}_{mn}^\theta = C_{mn}^\theta (\bar{f}_n - Z_{mn}) - C_{nm}^\theta (\bar{f}_m - Z_{nm}) \quad (3.117)$$

with

$$C_{mn}^\theta = \frac{h_{u,n}}{\Delta r_n} d_{nm} s_n^{mn}$$

$$C_{nm}^\theta = \frac{h_{u,n}}{\Delta r_n} d_{nm} s_m^{mn}$$

where

$$d_{nm} = [(a_n^{mn})^{-1} + (a_m^{mn})^{-1}]^{-1}$$

Note that the side-averaged currents in the azimuthal direction have been radially averaged, hence the $\frac{h_{u,n}}{\Delta r_n}$ term.

3.6.3 Tensorial source

The expressions obtained for the tensorial source in the v -direction are identical to those in the u -direction, with all parameters assuming their corresponding values in the v -direction.

$$Z_{mn}^{right} = \frac{(\frac{\eta h_u}{2})^2}{D_n (\beta_n^{nm})^2} \left(d_0 - \frac{1}{2} \sum_{l=0}^L d_l [\cosh(\beta_n^{nm}) f_l^{cos} + \sinh(\beta_n^{nm}) f_l^{sin}] \right) \quad (3.118)$$

$$Z_{mn}^{left} = \frac{(\frac{\eta h_u}{2})^2}{D_n (\beta_n^{nm})^2} \left(d_0 - \frac{1}{2} \sum_{l=0}^L d_l [\cosh(\beta_n^{nm}) f_l^{cos} - \sinh(\beta_n^{nm}) f_l^{sin}] \right) \quad (3.119)$$

Impact of variable separation on tensorial definition

We face here the identical situation as in the u -direction, needing to relate the one-dimensional average flux in θ to the node-averaged flux. We proceed similarly. We restate the relevant definitions:

$$\Phi_n(u, v) = f_n(u) + f_n(v) - \bar{f} \quad (3.120)$$

$$\bar{\Phi}_n = \frac{1}{h_u h_v} \int_{h_u} \int_{h_v} \Phi_n(u, v) g(u)^2 du dv \quad (3.121)$$

We utilize the relationship between $\bar{f}$ and $\bar{\Phi}_n$, since the side-averaged current to node-averaged flux relationship can only be found if it is known. As stated in eq. (3.117), we have:

$$\bar{J}_{mn}^\theta = C_{mn}^\theta (\bar{f}_n - Z_{mn}) - C_{nm}^\theta (\bar{f}_m - Z_{nm}) \quad (3.122)$$

Redefinition of tensorial source

Using eqs. (3.86) and (3.81) we may redefine the tensorial quantity as we did in the u -direction as follows:

$$\delta Z_{mn}^{right,left} = Z_{mn}^{right,left} + K \sum_{l=1}^{\infty} \frac{f_l^u g_l}{2^l + 1} \quad (3.123)$$

and remain with

$$\bar{J}_{mn}^\theta = C_{mn}^\theta (\bar{\Phi}_n - \delta Z_{mn}) - C_{nm}^\theta (\bar{\Phi}_m - \delta Z_{nm}) \quad (3.124)$$

This approach would once again successfully express the side-averaged current in terms of node-averaged flux, but is dependent upon the fact that the one-dimensional averages in u and v directions are equal. This might not be true at the start of the solution iteration process. On the other hand, if we once again consider the approach of separating the inhomogeneous source contribution (but now in v -direction) from the tensorial quantity in the v -direction, we may write:

$$Z_{mn}^{inh} = \frac{1}{2} \int_{-1}^1 (1 - \cosh(\beta_n^{nm} \pm \beta_n^{nm} w)) \left(\bar{f} - \frac{1}{2} \int_{-1}^1 g^2(u_n) f_n(u_n) du_n \right) dw \quad (3.125)$$

$$Z_{mn}^{inh} = (\bar{f}_u - \bar{\Phi}_n) + \left(-\frac{1}{2} \int_{-1}^1 \cosh(\beta_n^{nm} \pm \beta_n^{nm} w) (s_0^v) dw \right) \quad (3.126)$$

We may identify the first of these integrals as:

$$Z_{mn}^{inh,1} = \bar{f}_n - \bar{\Phi}_n \quad (3.127)$$

defining the remaining integral as:

$$Z_{mn}^{inh,2} = \left(-\frac{1}{2} \int_{-1}^1 \cosh(\beta_n^{nm} \pm \beta_n^{nm} w) \left(\bar{f} - \frac{1}{2} \int_{-1}^1 g^2(u_n) f_n(u_n) du_n \right) dw \right) \quad (3.128)$$

Replacing this definition within eq. (3.122), yields (once again denoting the tensorial contribution from other sources by Z_{mn}^{rem} i.e. $Z_{mn} = Z_{mn}^{rem} + Z_{mn}^{inh}$):

$$\bar{J}_{mn}^\theta = C_{mn}^\theta (\bar{\Phi}_n - (Z_{mn}^{inh,2} + Z_{mn}^{rem})) - C_{nm}^\theta (\bar{\Phi}_m - (Z_{nm}^{inh,2} + Z_{nm}^{rem})) \quad (3.129)$$

Relation (3.129) allows the definition of side-averaged currents in terms of node-averaged fluxes by limiting the contribution of the inhomogeneous source to the tensorial, and further limits the dependence of the numerical solution on calculated flux moments (especially from the moments in u -direction), which in turn depend, in the initial stages of calculation, on potentially disruptive initial guesses. The remaining component of the inhomogeneous source needs to be calculated, and evolves around the quantity:

$$Z_{mn}^{inh,2} = \left(-\frac{1}{2} \int_{-1}^1 \cosh(\beta_n^{nm} \pm \beta_n^{nm} w) \left(\bar{f} - \frac{1}{2} \int_{-1}^1 g^2(u_n) f_n(u_n) du_n \right) dw \right) \quad (3.130)$$

which may be written in terms of defined moments as:

$$Z_{mn}^{inh,2} = \frac{1}{2\sigma_n^{rem}} s_0^v [\cosh(\bar{\beta}_n^{nm}) f_0^{cos} + \sinh(\bar{\beta}_n^{nm}) f_0^{sin}] \quad (3.131)$$

3.7 Solution to the one-dimensional z -equation

The solution of the one-dimensional equation in the z -direction is identical to that of Cartesian coordinates as described in [11]. The one-dimensional, transversely integrated equation in the z -direction takes the form:

$$\frac{d^2}{dw^2} f_n(w) + (\beta_n^{nm})^2 f_n(w) = \frac{1}{-D_n} \left(\frac{h_{n,z}}{2} \right)^2 R_n(w) \quad (3.132)$$

with

$$(\beta_n^{nm})^2 = \left[\frac{\sigma_n^{rem} \left(\frac{h_{n,z}}{2} \right)^2}{-D_n} \right] \quad (3.133)$$

and

$$h_{n,z} = \Delta z_n$$

$$w = \frac{2z}{h_{n,z}}$$

$$R_n(w) = Q_n(w) - L_{n,z}(w)$$

The analytic solution to equation (3.132) is given by:

$$f_n(w) = C_{n,1} \cosh(\beta_n^{nm} w) + C_{n,2} \sinh(\beta_n^{nm} w) + \sum_{k=0}^L b_k P_k(w) \quad (3.134)$$

The particular solution was obtained directly from the source term by the following recursive relationship:

$$b_L = \frac{1}{(\beta_n^{nm})^2} \left(\frac{h_w}{2} \right)^2 D_n^{-1} d_L, \quad (3.135)$$

$$b_{L-1} = \frac{1}{(\beta_n^{nm})^2} \left(\frac{h_w}{2} \right)^2 D_n^{-1} d_{L-1}, \quad (3.136)$$

$$b_l = \frac{1}{(\beta_n^{nm})^2} \left[\left(\frac{h_w}{2} \right)^2 D_n^{-1} d_l - \sum_{m=l+2}^L a_{lm} b_m \right], \quad l = L-2, \dots, 1, 0 \quad (3.137)$$

with

$$a_{lm} = \frac{2l+1}{4} [1 + (-1)^{l+m}] [m(m+1) - l(l+1)] \quad (3.138)$$

These b_l coefficients are used in obtaining the expressions for c_1 and c_2 in eq. (3.134).

$$C_1 = \frac{(f^+ - Z^+) + (f^- - Z^-)}{2 \cosh(\beta_n^{nm})}$$

$$C_2 = \frac{(f^+ - Z^+) - (f^- - Z^-)}{2 \sinh(\beta_n^{nm})}$$

$$Z^+ = \sum_{k=0}^L b_k \quad (3.139)$$

$$Z^- = \sum_{k=0}^L b_k (-1)^k \quad (3.140)$$

$$f^+ = \phi_{n,n+1}^{mn} \quad (3.141)$$

$$f^- = \phi_{n,n-1}^{mn} \quad (3.142)$$

3.7.1 Determination of source moments

The total source moment in the z -direction is thus given as:

$$R_n(w) = Q_n(w) - L_{n,z}(w) = \sum_{l=0}^L R_l^z P_l(w) \quad (3.143)$$

with

$$L_n(w) = \sum_{l=0}^L l_l^z P_l(w)$$

$$Q_n(w) = Q_n^{fission}(w) + Q_n^{scatter}(w) + Q_n^{fixed} = \sum_{l=0}^L q_l^z P_l(w) \quad (3.144)$$

$$Q_n^{fission}(w) = \frac{1}{k_{eff}} \chi^g \sum_{h=1}^G v \sigma_{f,n}^h f^h(w)$$

$$Q_n^{scatter}(w) = \sum_{h=1, h \neq g}^G \sigma_{s0,n}^{h \rightarrow g} f^h(w)$$

Calculation of moments

In the z -direction only moments of the one-dimensional flux is required, and only for use in the fission and scattering sources. The definition and recurrence relations required are analogous to the development for the u -direction in Section 3.5.1, and will not be rederived here. Flux moments in the z -direction may then be expressed as:

$$f_l^z = \frac{2l+1}{2} \left(C_1 f_l^{z,cos} + C_2 f_l^{z,sin} \right) + b_l \quad (3.145)$$

Final form of source moments

Scattering source moments

$$q_l^{scatter} = \sum_{h=1, h \neq g}^G \sigma_{s0,n}^{h \rightarrow g} ((f)_l^h) \quad (3.146)$$

Fission source moments

$$q_l^{fission} = \frac{1}{k_{eff}} \chi^g \sum_{h=1}^G v \sigma_{f,n}^h ((f)_l^h) \quad (3.147)$$

Fixed source moment expression

The moments for the fixed source term may be expressed as

$$q_n^z = Q_n^{fixed} \quad (3.148)$$

Transverse leakage moment expression

The transverse leakage moments are defined across multiple nodes, and their treatment is left for Section 3.9.

3.7.2 Current and flux expressions

Using the one-dimensional analytic solution over multiple nodes, two important expressions are obtained. The first for surface-averaged current, and the second an expression for determining side-fluxes:

$$\bar{J}_{mn} = d_n^{mn} s_n^{mn} [\bar{\Phi}_n - Z_{mn}] - d_n^{mn} \phi_{n,m}^{mn} \quad (3.149)$$

which we may rewrite to solve for side-averaged flux as

$$\phi_{n,m}^{mn} = s_n^{mn} [\bar{\Phi}_n - Z_{mn}] - \frac{\bar{J}_{mn}}{d_n^{mn}} \quad (3.150)$$

with

$$Z_{mn} = \frac{(\frac{h_z}{2})^2}{-2(\beta_n^{mn})^2} \int_{-1}^1 (1 - \cosh(\beta_n^{mn} \pm \beta_n^{mn} w)) R_n(w) dw \quad (3.151)$$

$$t_n^{mn} = \frac{\bar{\beta}_n^{mn}}{\tanh(\beta_n^{mn})}$$

$$d_n^{mn} = (\frac{2}{h_z}) D_n t_n^{mn}$$

$$s_n^{mn} = \frac{2\bar{\beta}_n^{mn}}{\sinh(2\beta_n^{mn})}$$

These expressions culminate into the required surface-averaged current to node-averaged flux relationship in the z -direction:

$$\bar{J}_{mn} = C_{mn}^z (\bar{\Phi}_n - Z_{mn}) - C_{mn}^z (\bar{\Phi}_m - Z_{nm}) \quad (3.152)$$

with

$$C_{mn}^z = d_{nm} s_n^{mn}$$

$$C_{nm}^z = d_{nm} s_m^{mn}$$

where

$$d_{nm} = [(d_n^{mn})^{-1} + (d_m^{mn})^{-1}]^{-1}$$

Stating the relationship between scaled and unscaled currents for clarity:

$$\bar{J}_{n-1,n}^z = \frac{h_z}{2} J_{n-1,n} \quad (3.153)$$

$$\bar{J}_{n,n+1}^z = \frac{h_z}{2} J_{n,n+1}$$

3.7.3 Tensorial source

The expressions obtained for the tensorial source in the z -direction are identical to those in the u -direction, with all parameters defined as they are in the equations for z .

$$Z_{mn}^{right} = \frac{(\frac{h_z}{2})^2}{D_n(\beta_n^{nm})^2} \left(d_0 - \frac{1}{2} \sum_{l=0}^L d_l [\cosh(\beta_n^{nm}) f_l^{cos} + \sinh(\beta_n^{nm}) f_l^{sin}] \right) \quad (3.154)$$

$$Z_{mn}^{left} = \frac{(\frac{h_z}{2})^2}{D_n(\beta_n^{nm})^2} \left(d_0 - \frac{1}{2} \sum_{l=0}^L d_l [\cosh(\beta_n^{nm}) f_l^{cos} - \sinh(\beta_n^{nm}) f_l^{sin}] \right) \quad (3.155)$$

3.8 Balance equation

After quite some algebraic effort we have derived surface-averaged net current to node-averaged flux relationships for all three directions. In the case of r and θ directions, the relationship was indirectly obtained via the conformal mapping technique, while for z the approach was as it is normally done within the Analytic Nodal Method. All six relationship are finally inserted into the balance equation (eq. 3.2). Eq. (3.156) presents the final form of the balance equation for each node n . Note that the surfaces ($m = 1, 2 \dots 6$) are numbered as radial (inner, outer), azimuthal(right, left) and axial(bottom, top). Therefore, for example, $C_{z,n}^*$ would refer to the outer radial coupling coefficient of node n , and was defined in eq. (3.74).

$$\left[\sum_{m=1}^6 a_n^{nm} C_{mn} + \sigma_n^{ren} \right] \bar{\Phi}_n - \sum_{m=1}^6 a_n^{nm} C_{nm} \bar{\Phi}_m = \sum_{m=1}^6 a_n^{nm} [C_{mn} Z_{mn} - C_{nm} Z_{nm}] + \quad (3.156)$$

$$\frac{1}{k_{eff}} \chi^g \sum_{h=1}^G v^g \sigma_{f,n}^h (\bar{\Phi}_n) + \sum_{h=1, h \neq g}^G \sigma_{g,n}^{h \rightarrow g} (\bar{\Phi}_n)$$

3.9 Transverse leakage approximation

We conclude this chapter by formulating expressions for the transverse leakage terms in all three directions. The transverse leakage terms appeared as sources in all three one-dimensional equations, and expressions have to be developed for each of these. This section is handled here, at the conclusion of the chapter, since it requires developed net current expressions for all three directions. In this section both a flat and quadratic approximation will be developed, with the latter symbolizing a **new contribution for nodal methods in cylindrical geometry**. Within equation (3.57), (3.105) and (3.143) we face expressions for the transverse leakage for respectively u , v and z directions. In each of these cases we require one-dimensional currents on "top" and "bottom" surfaces in each transverse direction, which we do not have expressions for from the nodal solution. We do however have surface-averaged net currents on all transverse surfaces, and these currents can be used to construct a one-dimensional transverse leakage representation in an approximate way. Once a one-dimensional transverse leakage term is found, the analytic solution of the one-dimensional equations may be written in terms of these functions.

z-direction

Let us start by considering the equation in the z -direction (eq. 3.46). If we assume that radial and azimuthal currents are constant in the z -direction within each node, we can calculate the average transverse leakage in the z direction as

$$\bar{L}_{n,z} = \frac{1}{h_z} \int_{h_z} L_{n,z}(z) dz = \frac{J_{n,r}(r_n^-) + J_{n,r}(r_n^+)}{\Delta r_n} + \frac{J_{n,\theta}(\theta_n^-) + J_{n,\theta}(\theta_n^+)}{r_{n,mid} \Delta \theta_n} \quad (3.157)$$

We know the quantities on the right hand side by assuming that the one-dimensional equations in the transverse directions were solved. it is important to note that what we calculate as currents from the solutions in the transverse directions are not directly radial and azimuthal currents, but u and v currents - therefore they are the currents in the mapped u and

v directions. We are thus required to map these currents back into r and θ — directions before using them to express the average transverse leakage in the z -direction. The expressions for current in the one-dimensional solutions, as well as the mapping of these currents back into r and θ , were given in Section 3.3.1.

From this point onwards, two approaches are possible. The first to be discussed constitutes the simplest and most approximate solution, namely the “flat leakage approximation”. Thereafter, the more accurate, but slightly more instability-prone “quadratic leakage approximation” will be discussed.

Flat leakage approximation

The flat leakage approximation maintains the average transverse leakage from each transverse direction, and uses only information from the node under consideration. Eq. (3.157) gives the expression for the average transverse leakage. The expressions on the right hand side are known and constitute the r and θ -currents in the original coordinate system. Therefore we express

$$L_{n,z}(z) = \bar{L}_{n,z}^r(z) + \bar{L}_{n,z}^\theta(z) = \bar{L}_{n,z} \quad (3.158)$$

Quadratic leakage approximation

In the case of the quadratic leakage approximation, we use expression (3.157) to calculate the average transverse leakage in each of the three neighbouring nodes in the z -direction, and assume a quadratic polynomial shape over these three nodes.

$$L_{n,z}(z) = q_{n,0}^z + q_{n,1}^z z + q_{n,2}^z z^2 \quad (3.159)$$

We solve for $q_{n,0}^z$, $q_{n,1}^z$ and $q_{n,2}^z$ using the following closed set of equations, since we now know the average leakages on the right hand side from eq. (3.157):

$$\begin{aligned} \frac{1}{h_{n-1,z}} \int_{h_{n-1,z}} L_{n,z}(z) dz &= \bar{L}_{n-1,z} \\ \frac{1}{h_{n,z}} \int_{h_{n,z}} L_{n,z}(z) dz &= \bar{L}_{n,z} \\ \frac{1}{h_{n+1,z}} \int_{h_{n+1,z}} L_{n,z}(z) dz &= \bar{L}_{n+1,z} \end{aligned}$$

The detailed solution expressions for the quadratic fit may be found in Appendix G, and

we find an expression for the one-dimensional transverse leakage source in terms of node sizes in the z -direction, as well as average leakages in the r and θ -directions. We apply this transverse leakage shape $L(z)$ only to node n . This method is clearly an approximation, since it is not certain that a second-order polynomial will physically represent the transverse leakage function. It is convenient to express the solutions of $L(z)$ in terms of Legendre polynomials (for consistency with other one-dimensional sources). Therefore we would like:

$$L_{n,z}(z) = \sum_{k=0}^2 l_k^z P_k(z)$$

Equating coefficients with eq. (3.159) we find:

$$l_0 = q_{n,0}^z + \frac{q_{n,2}^z}{3}, \quad l_1 = q_{n,1}^z, \quad l_2 = \frac{2q_{n,2}^z}{3} \quad (3.160)$$

v -direction

The process is similar in the u and v -directions, taking care to handle the currents from mapped and unmapped coordinates correctly. The transverse leakage term in the v -equation:

$$L_{n,v}(v) = \frac{J_u(\frac{h_u}{2}, v) + J_u(-\frac{h_u}{2}, v)}{h_u} + \frac{\frac{1}{h_u} \int_{h_u} g(u)^2 J_z(u, v, \frac{h_z}{2}) du + \frac{1}{h_u} \int_{h_u} g(u)^2 J_z(u, v, -\frac{h_z}{2}) du}{h_z} \quad (3.161)$$

We obtain the average transverse leakage in the v -direction (analogous to the z -direction transverse leakage):

$$\bar{L}_v = \frac{J_u(\frac{h_u}{2}) + J_u(-\frac{h_u}{2})}{h_u} + \frac{\frac{1}{h_u h_v} \int_{h_u h_v} g(u)^2 J_z(u, v, \frac{h_z}{2}) dudv + \frac{1}{h_u h_v} \int_{h_u h_v} g(u)^2 J_z(u, v, -\frac{h_z}{2}) dudv}{h_z} \quad (3.162)$$

The term $\frac{1}{h_u h_v} \int_{h_u h_v} g(u)^2 J_z(u, v, \pm \frac{h_z}{2}) dudv$ presents a problem and careful consideration of the term is required. Notice firstly that if we try to express the z -direction current in terms of mapped coordinates, we find:

$$\begin{aligned} J(\pm \frac{h_z}{2}) &= -D \frac{d}{dz} f_n(z) \Big|_{\pm \frac{h_z}{2}} = -D \frac{d}{dz} \left(\frac{1}{S_{r\theta}} \int_{S_{r\theta}} \Phi(r, \theta, z) r dr d\theta \right) \Big|_{\pm \frac{h_z}{2}} \\ &= -D \frac{d}{dz} \left(\frac{r_i r_{i+1}}{S_{r\theta}} \int_{S_{r\theta}} \Phi(r_{scale}, \theta, z) r_{scale} dr_{scale} d\theta \right) \Big|_{\pm \frac{h_z}{2}} \end{aligned}$$

$$\begin{aligned}
&= -D \frac{d}{dz} \left(\frac{r_i r_{i+1}}{S_{r\theta}} \int_{h_u h_v} \Phi(u, v, z) g(u)^2 du dv \right) \Big|_{\pm \frac{h_z}{2}} \\
&= K_n \left(\frac{1}{h_u h_v} \int_{h_u h_v} J_z(u, v, \pm \frac{h_z}{2}) g(u)^2 du dv \right)
\end{aligned} \tag{3.163}$$

with K defined as in eq. (3.24). The manipulation allows us to write:

$$J(\pm \frac{h_z}{2}) = K_n \frac{1}{h_u h_v} \int_{h_u h_v} g(u)^2 J_z(u, v, \pm \frac{h_z}{2}) du dv$$

Therefore we may rewrite the expression for the average transverse leakage in v -direction as:

$$\bar{L}_{n,v} = \bar{L}_{n,v}^u + \bar{L}_{n,v}^z = \frac{J_u(\frac{h_u}{2}) + J_u(-\frac{h_u}{2})}{h_u} + \frac{J_z(\frac{h_z}{2}) + J_z(-\frac{h_z}{2})}{K_n h_z} \tag{3.164}$$

Flat leakage approximation

Once again the flat leakage approximation entails the calculation of only the average transverse leakage per node, and using that as a constant source term on the right hand side of the one-dimensional v -equation. We express:

$$L_{n,z}(v) = \bar{L}_{n,v}^u + \bar{L}_{n,v}^z = \bar{L}_{n,v} \tag{3.165}$$

Quadratic leakage approximation

The transverse currents on the right hand side are once again known from the solution of the one-dimensional equations in the u and z -directions. From here the process is identical in nature to the z -direction treatment, ending with an expression of the one-dimensional transverse leakage in terms of Legendre polynomials. We approximate as before:

$$L_{n,v}(v) = q_{n,0}^v + q_{n,1}^v v + q_{n,2}^v v^2$$

and apply

$$\frac{1}{h_{n-1,v}} \int_{h_{n-1,v}} L_{n,v}(v) dz = \bar{L}_{n-1,v}$$

$$\frac{1}{h_{n,v}} \int_{h_{n,v}} L_{n,v}(v) dz = \bar{L}_{n,v}$$

$$\frac{1}{h_{n+1,v}} \int_{h_{n+1,v}} L_{n,v}(v) dz = \bar{L}_{n+1,v}$$

and equate coefficients as in expression (3.160) to write (coefficients once again solved according to solution in Appendix G):

$$L_{n,v}(v) = \sum_{k=0}^2 l_k P_k(v) \quad (3.166)$$

***u*-direction**

The solution in the *u*-direction is slightly different. The inhomogeneous scaling function $g(u)^2$ does not integrate out in the *u*-direction, and we have the following expression for the transverse leakage (from eq.(3.28)):

$$L_{n,u}(u) = L_{n,u}^v(u) + g(u)^2 L_{n,u}^z(u) = \frac{J_v(u, \frac{h_v}{2}) + J_v(u, -\frac{h_v}{2})}{h_v} + g(u)^2 \frac{J_z(u, \frac{h_z}{2}) + J_z(u, -\frac{h_z}{2})}{h_z} \quad (3.167)$$

In this case we may approximate the transverse leakage component in the axial direction in three ways, and will present the first and third approaches in this section. We may aim to:

1. Use the flat leakage approximation.
2. Approximate, with a quadratic polynomial, the “transformed axial component of the transverse leakage”: $\frac{J_z(u, \frac{h_z}{2}) + J_z(u, -\frac{h_z}{2})}{h_z}$. This approach could potentially generate higher order terms, but will add complexity which might not add to the computational accuracy. The evaluation of this approach will not be further investigated within this thesis, and it is left as potential future work.
3. Approximate, with a quadratic polynomial, the “original axial component of the transverse leakage”: $g(u)^2 \frac{J_z(u, \frac{h_z}{2}) + J_z(u, -\frac{h_z}{2})}{h_z}$. This is the preferred implementation of quadratic leakage in the *u*-direction, and will be further developed in this section.

We proceed by obtaining average transverse leakages in the *u*-direction:

$$\bar{L}_{n,u} = \frac{J_v(\frac{h_v}{2}) + J_v(-\frac{h_v}{2})}{h_v} + \int_{h_u} g(u)^2 \frac{J_z(u, \frac{h_z}{2}) + J_z(u, -\frac{h_z}{2})}{h_z} du$$

and write analogously to 3.163:

$$\bar{L}_{n,u} = \frac{J_v(\frac{h_v}{2}) + J_v(-\frac{h_v}{2})}{h_v} + \frac{J_z(\frac{h_z}{2}) + J_z(-\frac{h_z}{2})}{K_n h_z} \quad (3.168)$$

$$\bar{L}_{n,u} = \bar{L}_{n,u}^v + \bar{L}_{n,u}^z$$

Flat leakage approximation

This is once again the simplest case, utilizing only the average of each transverse direction's contribution to the u -direction. Note that the contribution from z to u is identical to the average contribution from z to v as found in the previous section. We may write:

$$L_{n,u}(u) = \bar{L}_{n,u} \quad (3.169)$$

Quadratic leakage (original axial component)

In this approach we would approximate the one-dimensional transverse leakage shape, namely:

$$L_{n,u}(u) = L_{n,u}^v(u) + g(u)^2 L_{n,u}^z(u) \quad (3.170)$$

by

$$L_{n,u}(u) = q_{n,0} + q_{n,1}u + q_{n,2}u^2 \quad (3.171)$$

with $L_{n,u}(u)$ fitted in the normal way to conserve the average transverse leakage. Substituting eq. (3.168) for the average transverse leakage in the u -direction into the set below, and solving the set of equations once again as described in Appendix G:

$$\frac{1}{h_{n-1,v}} \int_{h_{n-1,v}} L_{n,u}(u) dz = \bar{L}_{n-1,u}$$

$$\frac{1}{h_{n,v}} \int_{h_{n,v}} L_{n,u}(u) dz = \bar{L}_{n,u}$$

$$\frac{1}{h_{n+1,v}} \int_{h_{n+1,v}} L_{n,u}(u) dz = \bar{L}_{n+1,u}$$

After obtaining the $q_{n,i}$ coefficients, we can express them as Legendre polynomial expansion coefficients using (3.160) for node n :

$$L_{n,u}(u) = \sum_{k=0}^2 l_k P_k(u)$$

3.10 Conclusion

This concludes the discussion on the development of the conformal mapping approach to the Analytic Nodal Method. The chapter followed the derivation to the point of expressing

all terms in the within-group diffusion balance equation in terms of the primary unknown, namely node-averaged flux. Utilizing appropriate boundary conditions, the set of equations are closed and may be solved numerically. The major obstacle, of not being able to obtain the necessary auxiliary one-dimensional θ -equation in cylindrical geometry, was circumvented by performing the transverse integration in mapped (u, v) Cartesian geometry. Some assumptions were introduced in this process, such as the separation of variables for the sake of constructing the sources terms in the v -equation, or the truncation of the Legendre source expansions after L terms (in practice to be implemented as 4 for the sake of the test code). These issues will be numerically evaluated in the upcoming results chapters, and further conclusions regarding their relevance will be drawn.

This chapter serves as the basis for the development of a numerical FORTRAN code to demonstrate the viability of this approach, and serves as a prototype for a possible future implementation into the Ncsa developed OSCAR code system [22]. Before describing the developed test code (Chapter 5) the next chapter will establish whether an important requirement of nodal methods is met by the conformal mapping approach, namely whether or not a fine-mesh limit exists for the expressions obtained in this chapter. This property is important, and directly relates the numerical stability of the solution algorithm to be implemented.

Chapter 4

FINE-MESH LIMIT

4.1 Introduction

The previous chapter concluded the development of the analytic nodal method in cylindrical geometry. Prior to that, in Chapter 2, the development of the finite-difference solution method was described. We now proceed to illustrate an important link between these two developments, by deriving the fine-mesh limiting expressions for the analytic nodal method. A necessary and important requirement of nodal methods in general is the existence of such a fine-mesh limit, which specifically refers to the property of equivalence of nodal equations and finite-difference equations in the limit of fine nodal meshes. This property is especially important for numerical stability of the nodal solution method and the ANM in Cartesian coordinates exhibits this property [11]. This chapter addresses the question as to whether or not the conformal mapping adjustments to the ANM maintains the fine-mesh limit property.

A given nodal method may be said to exhibit a fine-mesh limit if the balance equation, and hence node-averaged flux solution, is equivalent to the finite-difference solution on the same sufficiently fine mesh. Therefore, we must show that all terms in eq. (3.156) reduce to corresponding terms in eq. (2.14) in the limit of a fine-mesh, for one to be able to conclude that the conformal mapping approach to the analytic nodal method does exhibit a fine-mesh limit. In order to more clearly define the problem, we begin by attempting to restate these equations in reconciled notation.

The nodal balance equation, as derived in the previous chapter (eq. (3.156)) is given as:

$$\left[\sum_{m=1}^6 a_n^{nm} C_{mn} + \sigma_n^{rem} \right] \bar{\Phi}_n - \sum_{m=1}^6 a_n^{nm} C_{nm} \bar{\Phi}_m = \sum_{m=1}^6 a_n^{nm} [C_{mn} Z_{mn} - C_{nm} Z_{nm}] + \quad (4.1)$$

$$\frac{1}{k_{eff}} \chi^s \sum_{h=1}^G \psi^s \sigma_{f,n}^h (\bar{\Phi}_n) + \sum_{h=1, h \neq g}^G \sigma_{s0,n}^{h \rightarrow g} (\bar{\Phi}_n)$$

If we substitute the expression for side-averaged net current in all three directions (3.152, 3.124 and 3.74) back into eq. (4.1), and multiply the equation by node volume, we obtain:

$$\sum_{j=1}^6 \bar{J}_{jn} S_{jn} - Q_n V_n + \sigma_n^{rem} \bar{\Phi}_n V_n = 0 \quad (4.2)$$

with the expression for net current in each direction restated for clarity:

$$\begin{aligned} \bar{J}_{nn}^r &= C_{nn}^r (\bar{\Phi}_n - Z_{nn}^r) - C_{nm}^r (\bar{\Phi}_m - Z_{nm}^r) \\ \bar{J}_{nn}^\theta &= C_{nn}^\theta (\bar{\Phi}_n - Z_{nn}^\theta) - C_{nm}^\theta (\bar{\Phi}_m - Z_{nm}^\theta) \\ \bar{J}_{nn}^z &= C_{nn}^z (\bar{\Phi}_n - Z_{nn}^z) - C_{nm}^z (\bar{\Phi}_m - Z_{nm}^z) \end{aligned} \quad (4.3)$$

We find that eq. (4.2) is of course identical to the balance equation for the finite-difference development (eq. (2.14)), with the exception that the net current expressions within the finite-difference formalism have the following form (from eq. (2.14)):

$$\begin{aligned} J_{nm}^r &= \tilde{d}_{nm}^r [\Phi_n - \Phi_m] \\ J_{nm}^\theta &= \tilde{d}_{nm}^\theta [\Phi_n - \Phi_m] \\ J_{nm}^z &= \tilde{d}_{nm}^z [\Phi_n - \Phi_m] \end{aligned} \quad (4.4)$$

We may now formulate the requirement for a fine-mesh limit. We have to show that eq. (4.3) reduces to eq. (4.4) in the limit of a small mesh size. We therefore aim to show that as $h_w \rightarrow 0$:

1. Nodal coupling coefficients tend to finite-difference coupling coefficients: $C_{nn}^w = C_{nm}^w = \tilde{d}_{nm}^w$.
2. Tensorial contributions tend to 0: $Z_{nm}^w = 0$

for all directions $w = \{r, \theta, z\}$

In the coming sections, we show that points 1. and 2. above are satisfied for all directions concerned. However, from the nature of the logarithmic mapping function the developed discretization scheme is not defined in the coordinate origin. This was clear from Section 3.3, and hence we may expect that a fine-mesh limit does not exist in the coordinate origin (or arbitrarily close to it). This is in fact the case, and we will illustrate this fact near the end of the chapter. The arguments presented in Sections 4.2, 4.3 and 4.4 are therefore derived for all regions excluding the center of the system.

4.2 Axial direction

In order to demonstrate that nodal coupling coefficients limit to finite-difference coefficients, we investigate the form of the nodal coupling coefficients. We will consider each direction in turn, and begin with the axial direction, since no mapping or scaling factors are introduced in the axial direction, as is the case in radial and azimuthal directions. As stated, we are assured that a fine-mesh limit does exist in Cartesian coordinates, and hence we are reasonably assured that the axial nodal equations would limit to their finite-difference counterparts.

Coupling coefficients

The nodal axial coupling coefficients on the interface between node n and node m were given, in Section 3.7, as:

$$\begin{aligned} C_{nn}^z &= d_{nm} s_n^{mn} \\ C_{nm}^z &= d_{nm} s_m^{mn} \end{aligned} \quad (4.5)$$

$$d_{nm} = [(d_n^{mn})^{-1} + (d_m^{mn})^{-1}]^{-1}$$

$$d_n^{mn} = \left(\frac{2}{h_z}\right) D_n t_n^{mn}$$

$$t_n^{mn} = \frac{\beta_n^{nm}}{\tanh(\beta_n^{nm})}$$

$$s_n^{mn} = \frac{2\beta_n^{nm}}{\sinh(2\beta_n^{nm})}$$

$$\beta_n^{nm} = \sqrt{\frac{\sigma_n^{rem}}{D_n}} \left(\frac{h_{n,z}}{2}\right)$$

Considering eq. (4.5), the following may be deduced as $h_z \rightarrow 0$:

1. $\beta_n^{nm} \rightarrow 0$
2. t_n^{mn} and $s_n^{mn} \rightarrow 1$
3. C_{nn}^z and $C_{nm}^z \rightarrow \frac{2 \frac{D_n}{h_{n,z}} \frac{D_m}{h_{m,z}}}{\frac{D_n}{h_{n,z}} + \frac{D_m}{h_{m,z}}} = \bar{d}_{nm}^z$ (see definition of finite-difference axial coupling coefficients in eq. (2.11))

We may therefore deduce that the axial nodal coupling coefficients correctly limit to finite-difference coupling coefficients.

Tensorial source

In order to determine the leading order term in the case of a fine-mesh limit for the tensorial quantity, its expression will be expanded in a Taylor series and examined. The original expression of the axial tensorial quantity was (eq. (3.154)):

$$Z_{nm}^z = \frac{(\frac{h_z}{2})^2}{-2D_n(\beta_n^{nm})^2} \sum_{l=0}^L d_l \int_{-1}^1 (1 - \cosh(\beta_n^{nm} \pm \beta_n^{nm} w)) P_l(w) dw \quad (4.6)$$

In order to investigate the behaviour of this quantity for a limiting mesh size, we expand the cosine term (which contains node size as an argument) in a Taylor series as follows:

$$\begin{aligned} \cos(\beta_n^{nm} \pm \beta_n^{nm} w) &= 1 + \frac{(\beta_n^{nm} \pm \beta_n^{nm} w)^2}{2!} + \frac{(\beta_n^{nm} \pm \beta_n^{nm} w)^4}{4!} + \dots \\ &= 1 + (\beta_n^{nm})^2 \left\langle \sum_{k=1}^{\infty} c_{2k} (1 \pm w)^{2k} \right\rangle \\ c_{2k} &= \frac{(\beta_n^{nm})^{2k-2}}{(2k)!} \end{aligned} \quad (4.7)$$

We may substitute expression (4.7) into eq. (4.6), and obtain:

$$\begin{aligned} \lim_{h_z \rightarrow 0} Z_{nm}^z &= \lim_{h \rightarrow 0} \left[h_z^2 \sum_{l=0}^L \sum_{k=1}^{\infty} (A_{kl}) \right] \\ A_{kl} &= \frac{d_l c_{2k}}{4D_n} \int_{-1}^1 (1 \pm w)^{2k} P_l(w) dw \end{aligned} \quad (4.8)$$

The calculation of the A_{kl} terms are not important here, but rather the fact that the expression of Z_{nm}^z has as minimum leading order term a quantity of order h^2 (A_{kl} terms are all of order 1 or higher orders of h). Therefore

$$\lim_{h_z \rightarrow 0} Z_{nm}^z = O[h_z^2]$$

From the above expression we may deduce that, since the leading order term in the expansion is of order h^2 , the tensorial quantity in axial direction does approach zero in the limit of the fine-mesh, and furthermore does so according to the square of the mesh size.

This concludes the fine-mesh limit requirement for the equations in the axial direction, since the coupling coefficients limit to their finite-difference counterparts and tensorial quantities limits to zero. The result in this section is by no means unexpected, since the solution in axial direction is identical to that in Cartesian coordinates, where a fine-mesh limit ex-

ists for all directions [11]. We may proceed to investigate both the radial and azimuthal directions.

4.3 Radial direction

We will follow an analogous approach as in Section 4.2, investigating the behaviour of coupling coefficients and tensorial sources, but in this instance associated with the radial direction. We reiterate here that r is finite and non-zero, and hence this section relates to obtaining a fine-mesh limit in all regions of the system excluding the coordinate origin.

Coupling coefficients

The nodal radial coupling coefficients on the interface between node n and node m were given, in Section 3.5, as:

$$\begin{aligned} C_{mn}^r &= \frac{1}{r_{mn}} d_{nm} s_n^{mn} \\ C_{nm}^r &= \frac{1}{r_{mn}} d_{nm} s_m^{mn} \end{aligned} \quad (4.9)$$

$$d_{nm} = [(a_n^{mn})^{-1} + (a_m^{mn})^{-1}]^{-1}$$

$$a_n^{mn} = \left(\frac{2}{h_u}\right) D_n t_n^{mn}$$

$$t_n^{mn} = \frac{\overline{\beta_n^{nm}}}{\tanh(\overline{\beta_n^{nm}})}$$

$$s_n^{mn} = \frac{2\overline{\beta_n^{nm}}}{\sinh(2\overline{\beta_n^{nm}})}$$

$$(\beta_n^{nm})^2 = \left[\frac{\sigma_n^{rem} \left(\frac{\eta_n b_n}{2}\right)^2}{D_n} \right] \quad (4.10)$$

where

$$\eta^2 = r_i r_{i+1}$$

and

$$h_u = \ln(r_{i+1}) - \ln(r_i) = \ln\left(\frac{r_{i+1}}{r_i}\right) \quad (4.11)$$

We need to evaluate the behaviour of the coupling coefficients as $\Delta r \rightarrow 0$, and we begin by investigating the buckling term β_n^{nm} .

$$\lim_{\Delta r \rightarrow 0} \beta_n^{nm} = \lim_{\Delta r \rightarrow 0} \left[\sqrt{\frac{\sigma_n^{nm}}{D_n}} \frac{\sqrt{r_i(r_i + \Delta r)}}{2} \ln \left(\frac{r_i + \Delta r}{r_i} \right) \right] = 0 \quad (4.12)$$

The above limit is clearly zero when r_i is non-zero. We will investigate the result as r_i approaches zero in Section 4.5. Furthermore, if we consider the behaviour of the mapped node size as it appears in the expression for the coupling coefficient, we have

$$\lim_{\Delta r \rightarrow 0} h_u = \lim_{\Delta r \rightarrow 0} \ln \left(1 + \frac{\Delta r}{r} \right) = \lim_{\Delta r \rightarrow 0} \frac{\Delta r}{r} = 0 \quad (4.13)$$

With these results from eqs. (4.13) and (4.12) in mind, we may deduce that as $\Delta r \rightarrow 0$:

1. $\beta_n^{nm} \rightarrow 0$
2. t_n^{nm} and $\delta_n^{nm} \rightarrow 1$
3. C_{mn}^r and $C_{nm}^r \rightarrow \frac{2 \frac{D_n}{\Delta r_n} \frac{D_m}{\Delta r_m}}{\frac{D_n}{\Delta r_n} + \frac{D_m}{\Delta r_m}} = \tilde{d}_{nm}^r$ (see definition of finite-difference radial coupling coefficients in eq. (2.11))

We may therefore deduce that the radial nodal coupling coefficients correctly limit to finite-difference coupling coefficients.

Tensorial source

In order to determine the leading order term in the case of a fine-mesh limit for the radial tensorial quantity, we follow an analogous approach to the tensorial in the axial direction. The original expression of the radial tensorial quantity is:

$$Z_{mn}^r = \frac{(\frac{\eta h_u}{2})^2}{-2(\beta_n^{nm})^2 D_n} \int_{-1}^1 (1 - \cosh(\beta_n^{nm} \pm \beta_n^{nm} w)) R_n(w) dw \quad (4.14)$$

We employ an identical expansion as in eq. (4.7), and substitute it into eq. (4.14) to obtain:

$$\lim_{\Delta r \rightarrow 0} Z_{nm}^r = \lim_{\Delta r \rightarrow 0} \left[\eta^2 h_u^2 \sum_{l=0}^L \sum_{k=1}^{\infty} (A_{kl}) \right] \quad (4.15)$$

$$A_{kl} = \frac{d_l c_{2k}}{4 D_n} \int_{-1}^1 (1 \pm w)^{2k} P_l(w) dw$$

The quantity $\eta^2 h_u^2$ does limit to zero (from eq. (4.12)), and hence we are sure that the tensorial vanishes for small mesh sizes. Therefore

$$\lim_{\Delta r \rightarrow 0} Z_{nm}^r = O[h_u^2] = O[\Delta r^2]$$

From the above expression we may deduce that, since the leading order term in the expansion is of order h^2 , the tensorial quantity in radial direction does approach zero in the limit of the fine-mesh. This concludes the fine-mesh limit requirement for the equations in the radial direction, since the coupling coefficients limit to their finite-difference counterparts and the tensorial quantity limits to zero.

4.4 Azimuthal direction

Once more we follow an analogous approach as in Section 4.2, and investigate the behaviour of azimuthal coupling coefficients and tensorial sources.

Coupling coefficients

The nodal azimuthal coupling coefficients on the interface between node n and node m were given, in Section 3.6, as:

$$\begin{aligned} C_{mn}^\theta &= \frac{h_{u,n}}{\Delta r_n} d_{nm} s_n^{mn} \\ C_{nm}^\theta &= \frac{h_{u,n}}{\Delta r_n} d_{nm} s_m^{mn} \end{aligned} \quad (4.16)$$

$$d_{nm} = [(d_n^{nm})^{-1} + (d_m^{nm})^{-1}]^{-1}$$

$$d_n^{nm} = \left(\frac{2}{h_e}\right) D_n t_n^{nm}$$

$$t_n^{nm} = \frac{\overline{\beta_n^{nm}}}{\tanh(\overline{\beta_n^{nm}})}$$

$$s_n^{mn} = \frac{2\overline{\beta_n^{nm}}}{\sinh(2\overline{\beta_n^{nm}})}$$

$$(\overline{\beta_n^{nm}})^2 = \left[\frac{\sigma_n^{rem} \left(\frac{\eta_n h_n}{2}\right)^2}{D_n K} \right] \quad (4.17)$$

where

$$\eta^2 = r_i r_{i+1}$$

$$h_v = \Delta\theta$$

$$K = \frac{h_u h_v r_i r_{i+1}}{S_n^{r\theta}} = \frac{h_u}{\sinh(h_u)}$$

and

$$h_u = \ln(r_{i+1}) - \ln(r_i) = \ln\left(\frac{r_{i+1}}{r_i}\right) \quad (4.18)$$

Note that the expressions in the azimuthal direction depend not only upon node size in the azimuthal direction, but are also related to radial node size. We should begin by investigating the coupling coefficient scaling term $\frac{h_{u,n}}{\Delta r_n}$ within the limit (once again to reiterate that this argument is valid for all regions excluding the center of the system):

$$\begin{aligned} \lim_{\Delta r \rightarrow 0} \frac{h_{u,n}}{\Delta r_n} &= \lim_{\Delta r \rightarrow 0} \frac{1}{\Delta r_n} \ln\left(1 + \frac{\Delta r_n}{r_i}\right) \quad (4.19) \\ &= \lim_{\Delta r \rightarrow 0} \frac{1}{\Delta r_n} \ln\left(1 + \frac{\Delta r_n}{\bar{r}_i - \frac{\Delta r_n}{2}}\right) = \lim_{\Delta r \rightarrow 0} \frac{1}{\Delta r_n} \ln\left(1 + \frac{\Delta r_n}{\bar{r}_i} \frac{1}{1 - \frac{\Delta r_n}{2\bar{r}_i}}\right) \\ &= \lim_{\Delta r \rightarrow 0} \frac{1}{\Delta r_n} \ln\left(1 + \frac{\Delta r_n}{\bar{r}_i} \left(1 + \left[\frac{\Delta r_n}{2\bar{r}_i}\right] + \left[\frac{\Delta r_n}{2\bar{r}_i}\right]^2 + \left[\frac{\Delta r_n}{2\bar{r}_i}\right]^3 + \dots\right)\right) \\ &= \lim_{\Delta r \rightarrow 0} \frac{1}{\Delta r_n} \ln\left(\left(1 + \frac{\Delta r_n}{\bar{r}_i}\right) + O\left[\frac{\Delta r_n}{\bar{r}_i}\right]^2\right) = \frac{1}{\bar{r}_i} + O\left[\frac{\Delta r_n}{\bar{r}_i^2}\right] \end{aligned}$$

We may therefore deduce that as $\Delta\theta \rightarrow 0$ and $\Delta r \rightarrow 0$:

1. $\frac{1}{K} \rightarrow 1$
2. $\beta_n^{rm} \rightarrow 0$
3. β_n^{rm} and $s_n^{rm} \rightarrow 1$
4. C_{mn}^θ and $C_{nm}^\theta \rightarrow \frac{2 \frac{D_n}{\bar{r}_n \Delta \theta_n} \frac{D_m}{\bar{r}_m \Delta \theta_m}}{\frac{D_n}{\bar{r}_n \Delta \theta_n} + \frac{D_m}{\bar{r}_m \Delta \theta_m}} = \tilde{a}_{nm}^\theta$ (see definition of finite-difference radial coupling coefficients in eq. (2.11))

We may therefore deduce that the azimuthal nodal coupling coefficients correctly limit to finite-difference coupling coefficients.

Tensorial source

In order to determine the leading order term in the case of a fine-mesh limit for the azimuthal tensorial quantity, we follow an analogous approach to the tensorial in the radial direction. The original expression of the azimuthal tensorial quantity is:

$$Z_{nm}^\theta = \frac{(\frac{\eta h_v}{2})^2}{-2(\beta_n^{nm})^2 D_n} \int_{-1}^1 (1 - \cosh(\beta_n^{nm} \pm \beta_n^{nm} w)) R_n(w) dw \quad (4.20)$$

We employ an identical expansion as in eq. (4.7), and substitute it into eq. (4.20) to obtain:

$$\lim_{\Delta\theta \rightarrow 0} Z_{nm}^\theta = \lim_{\Delta\theta \rightarrow 0} \left[\eta^2 h_v^2 \sum_{i=0}^L \sum_{k=1}^{\infty} (A_{ki}) \right] \quad (4.21)$$

$$A_{ki} = \frac{d_i c_{2k}}{4D_n} \int_{-1}^1 (1 \pm w)^{2k} P_i(w) dw$$

We may therefore once more deduce that

$$\lim_{\Delta\theta \rightarrow 0} Z_{nm}^\theta = O[h_v^2] = O[\Delta\theta^2]$$

From the above expression we may deduce that, since the leading order term in the expansion is of order h^2 , the tensorial quantity in azimuthal direction does approach zero in the limit of the fine-mesh. This concludes the fine-mesh limit requirement for the equations in the azimuthal direction, since the coupling coefficients limit to their finite-difference counterparts and tensorial quantities limit to zero.

4.5 Fine-mesh expressions in the center

Radial direction

If we consider the behaviour of the radial direction coupling coefficient expressions arbitrarily close to and in the coordinate origin, we have to begin by investigating the behaviour of both the buckling and node size terms in the case when r_i also approaches zero (analogous to equations (4.12) and (4.13), and the problem may then be formulated as:

$$\lim_{\Delta r \rightarrow 0, r_i \rightarrow 0} \beta_n^{nm} = \lim_{\Delta r \rightarrow 0, r_i \rightarrow 0} \left[\sqrt{\frac{\sigma_n^{rem} r_i}{D_n}} \frac{\sqrt{(1 + \frac{\Delta r}{r_i})}}{2} \ln \left(1 + \frac{\Delta r}{r_i} \right) \right] \quad (4.22)$$

leading us to three distinct cases:

- Δr approaches zero faster than r_i , and the limit is clearly zero.
- Δr approaches zero at the same rate as r_i , and the limit remains zero.
- r_i approaches zero faster than Δr , and since $\frac{\Delta r}{r_i} \gg 1$, the problem reduces to:

$$\lim_{\Delta r \rightarrow 0, r_i \rightarrow 0} \beta_n^{nm} = \lim_{\Delta r \rightarrow 0, r_i \rightarrow 0} \left[\sqrt{\frac{\sigma_n^{nm}}{D_n}} \frac{\sqrt{r_i \Delta r}}{2} \ln \left(\frac{\Delta r}{r_i} \right) \right]$$

Consider

$$I = \frac{\ln \left(\frac{\Delta r}{r_i} \right)}{(r_i \Delta r)^{-\frac{1}{2}}} = \sqrt{r_i} \frac{\ln(\Delta r)}{(\Delta r)^{-\frac{1}{2}}} - \sqrt{\Delta r} \frac{\ln(r_i)}{(r_i)^{-\frac{1}{2}}}$$

We apply L'Hospital's theorem to this expression. Firstly we note:

$$\lim_{x \rightarrow 0} \frac{\ln(x)}{x^{-\frac{1}{2}}} = \lim_{x \rightarrow 0} \frac{\frac{1}{x}}{-\frac{1}{2}x^{-\frac{3}{2}}} = -\lim_{x \rightarrow 0} 2\sqrt{x} = 0$$

and therefore find:

$$\lim_{\Delta r \rightarrow 0, r_i \rightarrow 0} I = \lim_{\Delta r \rightarrow 0} \frac{\ln(\Delta r)}{\Delta r^{-\frac{1}{2}}} \lim_{r_i \rightarrow 0} \sqrt{r_i} - \lim_{r_i \rightarrow 0} \frac{\ln(r_i)}{r_i^{-\frac{1}{2}}} \lim_{\Delta r \rightarrow 0} \sqrt{\Delta r} = 0 - 0 = 0$$

The limit of expression (4.12) is once again zero. We may then conclude that the limit of expressions (4.12) is zero for all cases, and hence:

$$\lim_{\Delta r \rightarrow 0} \beta_n^{nm} = 0 \text{ everywhere} \quad (4.23)$$

On the other hand, if we consider the node size term

$$\lim_{\Delta r \rightarrow 0} h_u = \lim_{\Delta r \rightarrow 0} \left(\ln \left(1 + \frac{\Delta r}{r} \right) \right) = \lim_{\Delta r \rightarrow 0} \frac{\Delta r}{r} = 0 \text{ if and only if } r > 0 \quad (4.24)$$

From eq. (4.24) we deduce that the coupling coefficients do not limit correctly to their finite-difference counterparts in the center of the system, and as expected we do not achieve a fine-mesh limit for the net current expressions in the radial direction.

Azimuthal direction

If we consider the limiting expression for azimuthal coupling coefficients in the center of the system, we have to investigate the expression as both Δr and r_i approach zero (analogous to expression (4.19)):

$$\lim_{\Delta r \rightarrow 0, r_i \rightarrow 0} \frac{h_{i,n}}{\Delta r_n} = \lim_{\Delta r \rightarrow 0, r_i \rightarrow 0} \frac{1}{\Delta r_n} \ln\left(1 + \frac{\Delta r_n}{r_i}\right)$$

In order to evaluate this limit, let $r_i = (\Delta r_n)^\varepsilon$, $\varepsilon > 0$, and consider the following three cases:

- $\varepsilon > 1$

$$I = \lim_{\Delta r \rightarrow 0, r_i \rightarrow 0} \frac{1}{\Delta r_n} \ln(1 + (\Delta r_n)^{1-\varepsilon}) \approx \lim_{\Delta r \rightarrow 0} (1 - \varepsilon) \frac{\ln(\Delta r_n)}{\Delta r_n} = \infty$$

- $\varepsilon = 1$

$$I = \lim_{\Delta r \rightarrow 0, r_i \rightarrow 0} \frac{\ln(2)}{\Delta r_n} = \infty$$

- $\varepsilon < 1$

$$I = \lim_{\Delta r \rightarrow 0, r_i \rightarrow 0} \frac{1}{\Delta r_n} \ln(1 + (\Delta r_n)^{1-\varepsilon}) \approx \lim_{\Delta r \rightarrow 0, r_i \rightarrow 0} \left(\frac{1}{\Delta r_n}\right)^\varepsilon = \infty$$

Hence $I \rightarrow \infty$ as both $r_i, \Delta r \rightarrow 0$. We once again have to conclude that a fine-mesh limit for the coupling coefficients does not exist in the center for the azimuthal equations.

4.6 Conclusion

This chapter addressed the existence of a fine-mesh limit for the nodal equations, or more precisely, the property of the nodal equations to yield finite-difference equivalent expressions for limiting mesh sizes. Two major conclusions may be drawn from this discussion:

- The nodal balance equation reduces to the finite-difference balance equation for small mesh sizes in all regions of the system excluding the center (or arbitrarily close to it). This result is important, since we may subdivide calculational meshes in the system and be sure that the accuracy would improve. The exclusion of the center is due to, and consistent with, the fact that the mapping function is not defined in the coordinate origin. Furthermore, some heuristic guidelines as to the distribution of inner mesh sizes may be deduced from the discussions in Section 4.5, in that inner mesh size (remembering that extra inner meshes are required due to nature of the inhomogeneous source) should be of the order of the absolute radial coordinate of the mesh (e.g. eq. (4.24)) to avoid potential numerical instabilities.
- The point above constitutes some further motivation concerning special treatment of the central region. In Chapter 3 the possibility of a central cut-out region, in

order to exclude the logarithmic singularity in the mapping function, was introduced. Results from the current chapter support such a suggestion, but provides another potential solution, in the form of a hybrid finite-difference/nodal solution method. A possible application of such an approach would be the use of finite-difference coupling coefficients near the center (within a couple of neutron path lengths), and the developed nodal solution method for the remainder of the system. Results further show that finite-difference coupling coefficients for such a central hybrid approach may have to be used explicitly, since the nodal coupling coefficients do not limit correctly to their finite-difference counterparts arbitrarily close to the center.

Chapter 5

NODAL CODE VALIDITY

5.1 Introduction

Two test codes were developed based upon the derived equations in Chapters 2 and 3, and the current chapter introduces the first numerical solutions utilizing these codes. The development of the proposed nodal method, and subsequent nodal test code, contain some models and assumptions which will have to be numerically justified. In this regard we may consider the approximation of the inhomogeneous mapping source by a Legendre polynomial expansion, and the inner cut-out approximation to avoid the singularity in the coordinate origin. In order to investigate the domain of applicability of these approximations, two test problems are defined and calculated, which respectively represent the ideal and worst case scenario for the proposed conformal mapping approach. The first is a homogeneous hollow cylinder problem, and the second a two-dimensional "striped" (r, θ) problem (see Figure 5.2). The definition and reasoning behind these problems are discussed later in this chapter. However, utilizing these problems, we are able to investigate the domain of relevancy of the proposed method, and make some decisions regarding areas of practical application and potential areas of future work. This chapter therefore serves as initial testing of the NoRTHZ code. Validation will thus begin by considering:

- the code **precision**, referring to correctness of implementation. The solution of the NoRTHZ code should, e.g., be exact for a hollow infinite cylinder problem, since no removal of the logarithmic singularity is necessary in this case. The current implementation places a small cut-out in the center of the system, with a reflective boundary condition placed on the edge of the cut-out region. The hollow cylinder problem should therefore be precisely and accurately calculated by both the nodal and finite-difference codes, and an analytic solution in terms of Bessel functions may be written to confirm

this.

- the code **accuracy**, referring to applicability and relevancy of assumptions. Here we refer to issues which may degrade the quality of the solution, such as the inner cut-out approximation, accuracy of solution near the center due to both a large inhomogeneous source contribution and/or azimuthal inhomogeneity near the center. Central azimuthal inhomogeneity, or any corner material discontinuity within a system, poses a challenge to both the nodal and finite-difference approaches, due to the corner singularity problem within the neutron diffusion equation. The analytic solution to this problem, described by Cacuci [23], is rather complex, and relates to the unbounded spatial derivative in the corner point. Here it is sufficient to note that even though a fine-mesh finite-difference solution will be inaccurate in the center of a system, the logarithmic singularity in the spatial derivative is mild in nature, and a reasonable result may still be expected.

We continue with a short description of the test codes which were developed in the course of this work, and which serve the purpose of numerically evaluating the proposed conformal mapping technique.

5.2 Test code description

- **SciFi** is a 3D cylindrical multi-group mesh-centered finite-difference code with mesh refinement. No outer acceleration is built into the code and limited inner acceleration exists (Gauss Seidel with relaxation). Results from SciFi will be considered as reference. The implemented solution proceeds in a group-by-group fashion, and hence upscattering iterations are implemented. More detail regarding the implementation was given in Chapter 2.
- **NoRTHZ** is a 3D cylindrical nodal (ANM) code, implementing the conformal mapping technique and represents and numerically describes the bulk of the developments in Chapter 3. The code performs both fixed source and multi-group eigenvalue calculations. Furthermore, both flat and quadratic leakage approximations have been implemented. The group-by-group solution is also implemented, and fission, scattering and inhomogeneous source terms are expanded in Legendre polynomial series (up to the fourth order). Since the mapping approach forces an exclusion of the coordinate origin, a small cut-out (1 cm) in the case of NoRTHZ is placed about the center. The flux in this region then has to be calculated via an alternative method. Two rudimentary methods are built into NoRTHZ, namely to approximate the center flux as

an azimuthally weighted average of first radial ring average fluxes, or an azimuthally weighted average of the first radial ring inner side fluxes (these are available from e.g. eq. (3.72) for the u side fluxes). More advanced methods are considered as future development. A final note regarding the implementation should relate to nesting of iteration levels. The standard nesting scheme regarding this class of nodal methods would contain (from inner to outer) flux solution iterations, the energy group loop, up-scattering source iterations, outer eigenvalue iterations and finally feedback iterations in the case where intra-nodal cross-section feedback is utilized (not implemented in NoRTHZ). In the case of the conformal mapping approach, a further non-linear source needs to be evaluated, namely the inhomogeneous geometric source which appears due to the geometric transformation. There are many options as to the placement of this iteration level, but for the sake of the test code an extra iteration level has been added outside of the inner flux iterations. This approach might not lead to optimized performance, but seems to improve stability.

Acceleration schemes within NoRTHZ are equivalent to those in SciFi, and hence valid timing comparisons between the two codes could be made. Absolute times reported in this work may realistically be reduced by a further factor of at least 20 when the methods are built into an appropriately accelerated code. Appropriate schemes would include Chebyshev Cyclic Semi Iterative (CCSI) for inner iterations and Wielandt shift acceleration for eigenvalue iterations. Confirming realistic calculational time is important and therefore the cylindrical ANM will be implemented into the Necsca developed MGRAC code [22] for this purpose.

5.3 Hollow cylinder problem

In order to validate the basic conformal mapping approach, we begin with a very simple hollow, infinite cylinder. Problem 1 represents a 15 cm radius, radially homogeneous, axially infinite cylinder, with a 1 cm cut-out in the center for the nodal calculation ($\sigma_r = 0.5 \text{ cm}^{-1}$, $D = 1 \text{ cm}$, $\nu\sigma_f = 0.5 \text{ cm}^{-1}$). Three classes of independent results are produced (the relative convergence criterion is set to 10^{-8} in flux):

- Reference finite-difference solution, with a 1 cm cut-out and accompanying internal boundary condition (zero current) at the edge of the cut-out. This result should match the nodal solution, since it is the precise problem solved by NoRTHZ. This result may be used to investigate the accuracy of the inhomogeneous source near the center of the system. This solution set, within Table 5.1 below, is termed **FD_CUT**.

- Fine-mesh finite-difference solution for a 15 cm system without a center cut-out - therefore a full axially infinite cylinder problem. This problem serves to quantify the error in introducing the cut-out, and defines a reference cut-out flux. This solution set is termed **FD_FULL**.
- Multiple sets of nodal solutions, utilizing three meshes. The first mesh is fixed at 1 cm for the inner cut-out, while the sizes of meshes two and three (zones 2 and 3 in the table) are parametrically varied. This solution set is termed **N(a,b)**, where (a,b) refers to the sizes of meshes 2 and 3 respectively. As example, N(4,10) refers to a nodal discretization with node sizes 1, 4 and 10 cm to cover the 15 cm system.

The analysis of these results aim to quantify the following:

- How severe is the 1 cm cut-out approximation for a problem which is small and homogeneous about the center, and do the implemented methods of estimating the cut-out zone flux produce reasonable results. In Table 5.1, *Inner Flux 1* refers to the cut-out zone flux based upon the node-averaged flux method, and *Inner Flux 2* to the method based upon inner side fluxes. These two approaches were described in Section 5.2.
- Which constraints apply to the choice of inner mesh sizes, given the fact that the inhomogeneous source is largest where the ratio of consecutive radial meshes is greatest.

Results of applying both the SciFi and NoRTHZ codes to the hollow cylinder problem are summarized in Table 5.1. In the table, FD_CUT serves as reference for the nodal calculation for the k_{eff} , *Zone 2 err* and *Zone 3 err* fluxes, and the reference solution for both *Inner flux 1* and *Inner flux 2* is given by the FD_FULL solution. All percentages in the table refer to relative percentage differences between the nodal and appropriate finite-difference solution. The final two entries in the table refer to nodal calculations with multiple nodes (four and fifteen nodes respectively).

Method	k-eff	Inner flux 1	Inner Flux 2	Zone 2 err	Zone 3 err
FD_FULL	0.9618551	5.2570	NA	NA	NA
FD_CUT	0.9613910 (48 pcm)	NA	NA	NA	NA
N(3,11)	0.9613916 (sub-pcm)	5.0065 (4.7%)	5.1474 (2.09%)	0.0022%	0.0003%
N(4,10)	0.9613917 (sub-pcm)	4.9038 (6.7%)	5.1474 (2.08%)	0.0020%	0.0005%
N(5,9)	0.9613918 (sub-pcm)	4.7764 (9.1%)	5.1474 (2.08%)	0.0020%	0.0007%
N(6,8)	0.9613919 (sub-pcm)	4.6260 (12%)	5.1475 (2.08%)	0.0020%	0.0011%
N(7,7)	0.9613921 (sub-pcm)	4.4525 (15.3%)	5.1477 (2.08%)	0.0022%	0.0019%
N(8,6)	0.9613924 (sub-pcm)	4.2634 (18.9%)	5.1480 (2.07%)	0.0024%	0.0028%
N(9,5)	0.9613930 (sub-pcm)	4.0550 (22.9%)	5.1485 (2.06%)	0.0026%	0.0045%
N(2,4,8)	0.9613917 (sub-pcm)	NA	NA	NA	NA
N(1,1,1..)	0.9613918 (sub-pcm)	NA	NA	NA	NA

Table 5.1: Nodal results for hollow cylinder problem

Some immediate conclusions may be drawn from the table above.

- Eigenvalues match between FD_CUT and all the nodal discretizations (sub-pcm errors). This indicates that the basic nodal methodology performs as expected.
- An eigenvalue comparison between FD_CUT (or nodal) and FD_FULL shows an error of 48 pcm due to the cut-out. Given that this is a neutronically small reactor problem, such a difference will become progressively smaller as the problem approaches realistic reactor sizes. This will be further illustrated in Chapter 6. Problems exhibiting inner azimuthal inhomogeneity may produce larger errors, and such a problem is investigated in Section 5.4.
- The inner flux approximation, utilizing the side flux method ("Inner Flux 2" in table), is more accurate in reproducing the cut-out-zone flux, especially when the inner mesh size grows. This is as expected, since the flux shape within the second mesh is taken into account.

The eigenvalue and zone flux errors for the given problem, with a fourth order expansion in the inhomogeneous source, are very small and it may be difficult to extract useful trends from the data. In order to draw conclusions concerning possible restrictions upon the inner meshing scheme, the above calculation is repeated with the **inhomogeneous source expansion limited to the second order**. Such a calculation would severely over emphasize any limitations due to the inhomogeneous source, or more directly, due to the conformal mapping approach, and hence allow as an heuristic evaluation of the behaviour of NoRTHZ.

Figure 5.1 highlights these error trends by plotting eigenvalue errors and zone flux errors (as compared to reference SciFi results) against various nodal discretizations (as in Table 5.1). The results from the second order expansion calculation are presented as a graph to highlight the fact that an optimum solution (point of minimum error) is obtained.

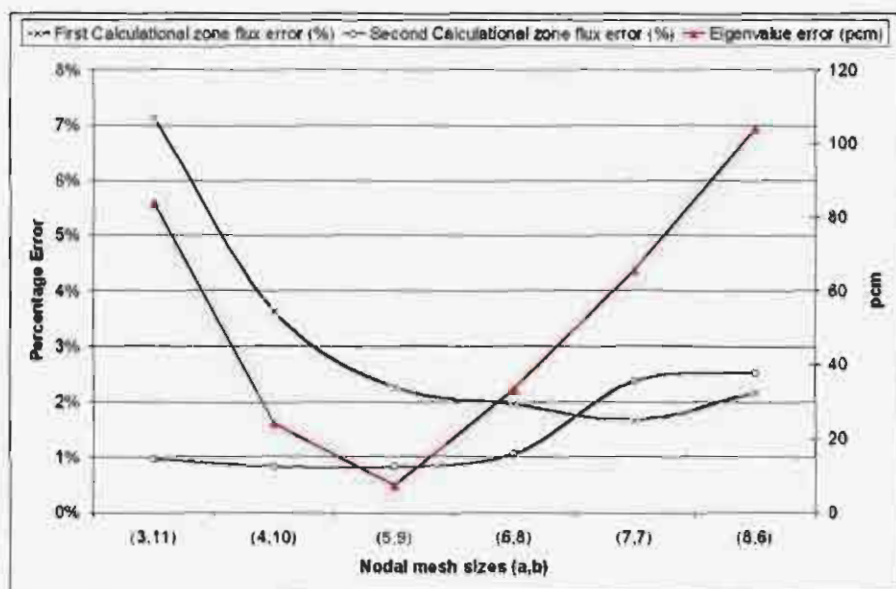


Figure 5.1: Infinite cylinder flux and eigenvalue error trends - 2nd order expansion

The following conclusions may be drawn from Figure 5.1:

- Errors are substantially larger for the case with only a second order expansion in the inhomogeneous source, with a couple of percent error in zone fluxes, and between 10 and 100 pcm in k_{eff} . This is due to the exponential nature of the inhomogeneous source and is clear from a comparison between the order of the errors in Figure 5.1 and those in Table 5.1.
- The error in eigenvalue is minimized for a balanced mesh distribution (case (5,9)). If the ratio of radial node boundaries are too large in either the inner or outer meshes, the solution degrades.

Although the hollow cylinder problem is a very simple construction, it allows us to investigate expected features of the method. The conclusion is drawn that practical problems might require more inner calculational meshes than the material distribution demands, and that

care must be taken in the choice of inner mesh sizes. We may consider some options in the choice of such inner meshing schemes:

- Equi-distant radial spacing. Such an approach would lead to an inner mesh of approximately 7 cm.
- Equi-volume radial spacing. This approach would lead to an inner mesh size of approximately 10.6 cm.
- Equi-logarithmic radial spacing. This would yield even sized meshes in mapped coordinates, and lead to an inner mesh choice of approximately 3.9 cm.

An investigation into the presented results in Figure 5.1 leads us to believe that the last option is preferable, since equi-logarithmic spacing (3.9 cm) is nearest to minimizing flux and eigenvalue errors. Such a conclusion is expected, since it would minimize the size of the average inhomogeneous source in the system; large inhomogeneous sources could expose truncation errors in the fourth order expansions implemented for these sources.

5.4 “Striped” (r, θ) problem

The problem in this section can be described as a potential worst-case formulation for this method, and will test the implementation much more severely. The problem will test the mapping approach in multidimensional (r, θ) coordinates, addressing issues such as azimuthal inhomogeneity in the center, as well as the importance of quadratic transverse leakage within cylindrical geometry. The (r, θ) “striped” problem is illustrated in Figure 5.2 below. This problem aims to:

- Apply the conformal mapping approach to a multidimensional (r, θ) problem. Figure 5.2 contains azimuthally alternating fuel ($\nu\sigma_f = 0.3$ cm, $\sigma_r = 0.2$ cm, $D = 1/\text{cm}$) and absorber ($\sigma_r = 0.5$ cm, $D = 1/\text{cm}$) regions.
- Investigate the accuracy of the flux distribution and cut-out zone flux approximation for a problem with azimuthal inhomogeneity, taking into account that the problem contains severe inhomogeneity in the coordinate origin.
- Test the flat and quadratic transverse leakage options developed within NoRTHZ.

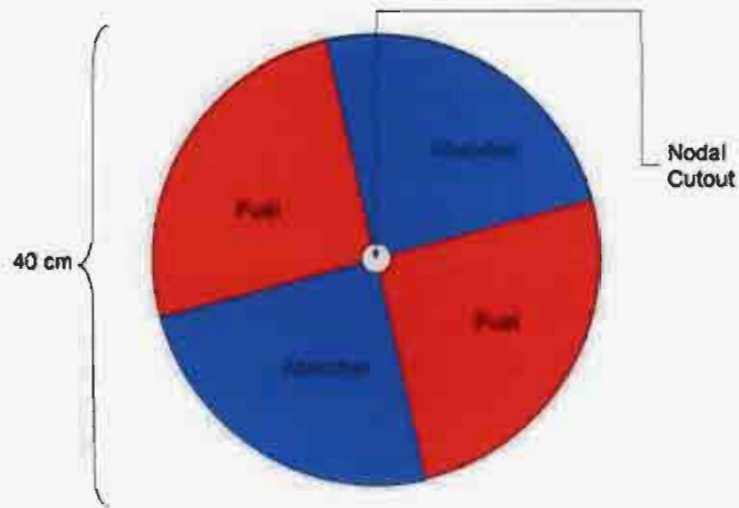


Figure 5.2: (r,θ) "Striped" problem geometric description

In order to understand the nature of the problem, the finite-difference solution is illustrated in Figure 5.3 and depicts radial flux profiles (arbitrary normalization) through both the source and absorber zones of Figure 5.2 (profiles represent the azimuthal averages over all finite-difference meshes within the zones).

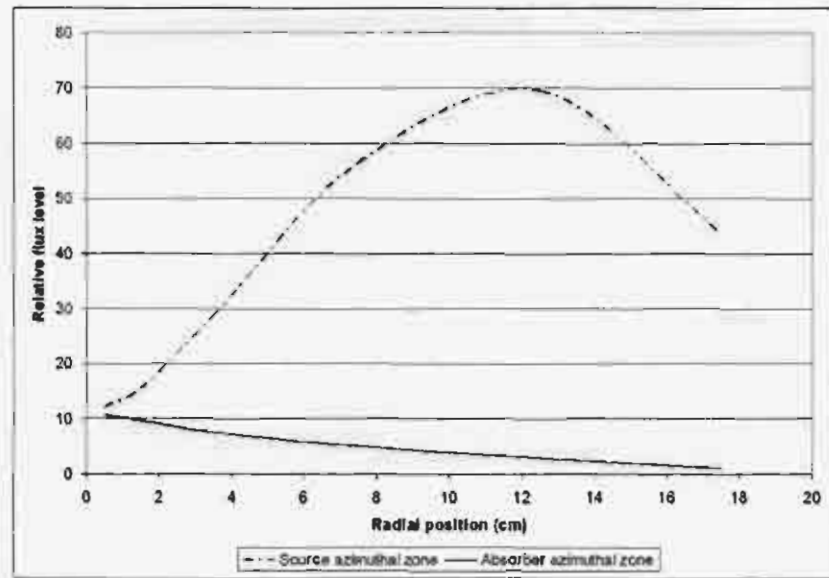


Figure 5.3: Reference solution for the "Striped" problem

We proceed and apply the NoRTHZ code to this problem. The cut-out indicated in Figure 5.2 is used within the NoRTHZ code, and the inner flux is approximated via the "inner side flux" method. Table 5.2 below presents global results for the problem, and shows eigenvalues and inner flux results for the following four cases:

1. **FD (ref)**: The reference finite-difference solution contains no cut-out.
2. **Nodal (flat)**: NoRTHZ calculation utilizing the flat leakage approximation
3. **Nodal (quad)**: NoRTHZ calculation utilizing the quadratic leakage approximation
4. **FD (cut-out)**: The finite-difference calculation for the problem which contains a cut-out. This result is added to provide some measure of the error introduced by adding the cutout (this may be seen by comparing FD (ref) to FD (cut-out)) . No inner flux result is of course available in this set.

Nodal results are calculated with the cut-out plus five radial (sizes of 1, 3, 5, 5, and 5 cm), and twelve azimuthal meshes (30 degrees per node). Finite-difference reference results are 30 times refined in both directions, as compared to the nodal sizes.

Result	FD (ref)	Nodal (flat)	Nodal (quad)	FD (cut-out)
k-eff	1.21999	1.22975 (800 pcm)	1.22167 (138 pcm)	1.22016 (14 pcm)
Inner flux	11.36714	12.16055 (7%)	13.03466 (14%)	NA

Table 5.2: "Striped" problem global results

The following global trends are observed:

- The accuracy of the nodal solution improves significantly with the use of quadratic leakage (800 pcm to 138 pcm), but an error of 138 pcm remains due to the inner inhomogeneity.
- Although the eigenvalue improves significantly with quadratic leakage, the azimuthally-averaged inner flux approximation becomes worse (14% error in inner zone average). This is an expected result due to the impact of the reflective boundary condition at 1 cm (from the solution in Figure 5.3 the flux is clearly not constant at 1 cm), which would distort the three-node radial transverse leakage fit from its true shape. A note is required here. The quadratic leakage approximation requires three nodes in order to complete the fit (Section 3.9), which are of course not available for boundary nodes. At these positions, and in this case for the zero net current (reflective) boundary condition in the center, an identical fictitious outer node is assumed to complete the fit. Such an assumption is consistent with the boundary condition, but propagates the error introduced by the inner boundary condition (which is non-physical) some distance into the system.

In order to investigate this further, Figures 5.4 and 5.5 show the radial profiles of the percentage flux error for both source and absorber azimuthal zones. The error is plotted for both the quadratic and flat leakage approximations. In Figures 5.4 and 5.5, errors are given by comparing nodal fluxes with reference finite-difference averages over the same nodal regions.

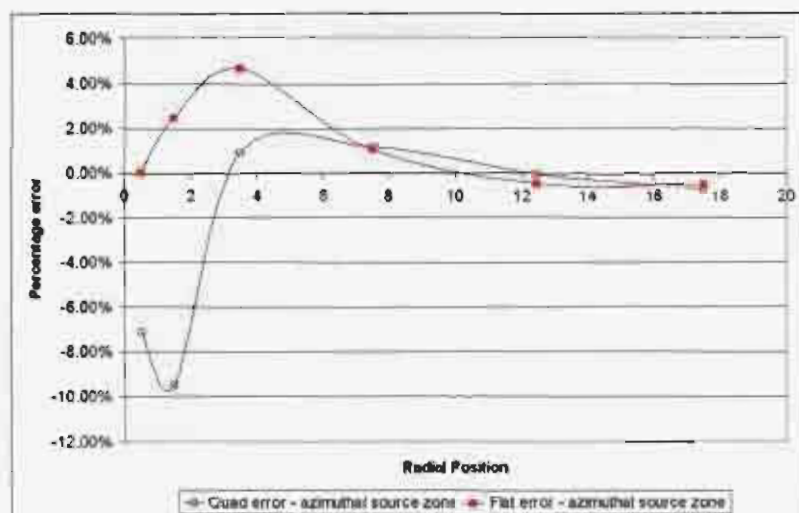


Figure 5.4: "Striped" problem flux error (radial profile) along source zone

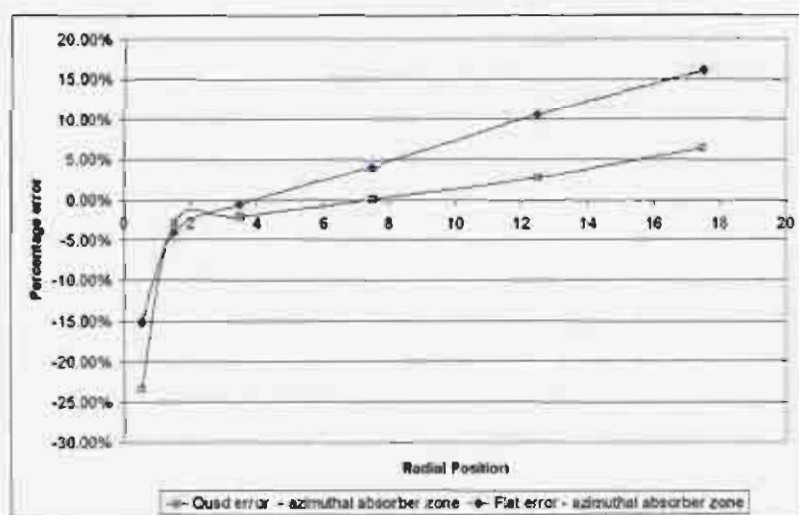


Figure 5.5: "Striped" problem flux error (radial profile) along absorber zone

The above figures support prior observations. The quadratic leakage approximation improves upon the percentage flux error within nearly all zones of the system, with the exception of the inner cut-out and the 2nd source zone. Within these inner regions, the zero net current boundary condition placed at the edge of the inner cut-out distorts the quadratic leakage shape. In this problem, therefore, the inner cut-out approximation impacts upon

the solution in two distinct ways, namely by homogenizing the central disc, and secondly by forcing a zero net current boundary condition at the edge of the central disc. In situations where these assumptions are violated and where the size of the inner disc is significant in comparison to the size of the system (as is the case in this problem), the method does lack in accuracy. In these cases improved methods for approximating the solution in the center have to be developed. Such approaches could include:

- An analytic solution for a homogenized central disc. Such an approach would still require smearing the azimuthal inhomogeneity, but would improve upon the flux profile vs. the zero net current boundary condition at the edge of the cut-out. A conformal mapping approach by mapping a circle into a rectangle would yield a similar solution. The simplest approach to yield a homogeneous solution might be a hybrid finite-difference / nodal formalism, utilizing a finite-difference approximation within the central disc, and applying appropriate interface conditions between finite-difference and nodal currents at the edge of the disc.
- A rigorous (analytically correct) (r, θ) solution, as proposed in [12] or [23], applied only to the center region. Although these solution methods are complex to implement, and may degrade performance, their limited use in the center of the system might be viable.

The results from this problem conclude this chapter on initial verification and investigation of the NoRTHZ code. Results were as expected for the two test problems and the implemented quadratic leakage approximation yields a dramatic improvement in eigenvalue, and similarly in node-averaged fluxes. The following chapter applies the NoRTHZ code to realistic reactor problems, and will show that the approximations in the development are not as limiting in these cases. Three reactor benchmark problems will be considered, and conclusions regarding accuracy and performance will be drawn.

Chapter 6

RESULTS AND DISCUSSION

6.1 Dodds' benchmark application

The first problem under discussion for the verification of the NoRTHZ code, is the benchmark problem published by Dodds in [7] and [8]. This problem also served as one of the verification problems for the SciFi finite-difference code in Chapter 2 and was described there. In this chapter, the 2D (r, z) Dodds' steady state configuration is used (depicted in Figure 2.2) to investigate the accuracy of the conformal mapping method. Since the model is (r, z) only, a single homogeneous azimuthal node is used and only conformal mapping effects with regard to the radial direction are considered. This represents a natural first test for the method. Table 6.1 below gives global eigenvalue results for the NoRTHZ vs SciFi codes as applied to Dodds' benchmark. In the table, the number of r and z meshes are given for each calculational case; we may see that the finite-difference ("FD") solution, as compared to the "Nodal large" solution, is approximately 8 times refined.

Method (r x z mesh points/nodes)	Eigenvalue (k_{eff})	Error (pcm)
FD (120x112)	0.868139	—
Nodal (quadratic leakage) (33x28)	0.868146	0.8
Nodal large (flat leakage) (16x14)	0.868282	16.4
Nodal large (quadratic leakage) (16x14)	0.868122	2

Table 6.1: Eigenvalue results for 2D Dodds' benchmark problem

We note from the above table that all the nodal results, especially the nodal cases utilizing quadratic leakage, demonstrate excellent agreement regarding eigenvalue. This is evident

from the "Nodal large" result which reaches an accuracy of 2 pcm. We further illustrate this problem by presenting axial and radial multi-group flux profiles, radially and axially-averaged respectively. Figures 6.1 and 6.2 present flux profiles from SciFi and NoRTHZ which have been normalized to the same arbitrary quantities and are hence termed "Relative flux". The nodal results represent region averages and the finite-difference profiles depict the actual point-wise flux profiles.

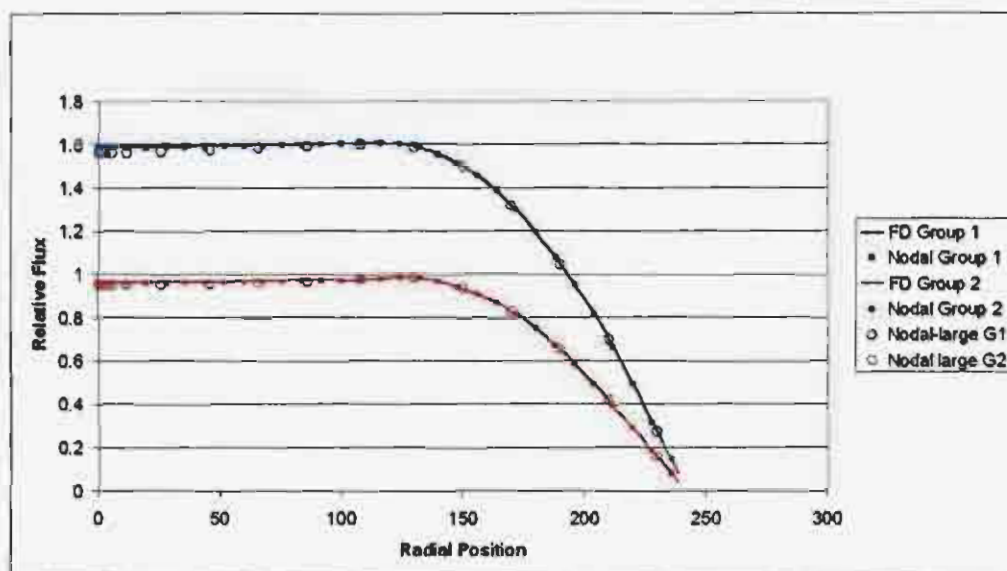


Figure 6.1: Dodds 2D (r, z) - radial profile (axially-averaged)

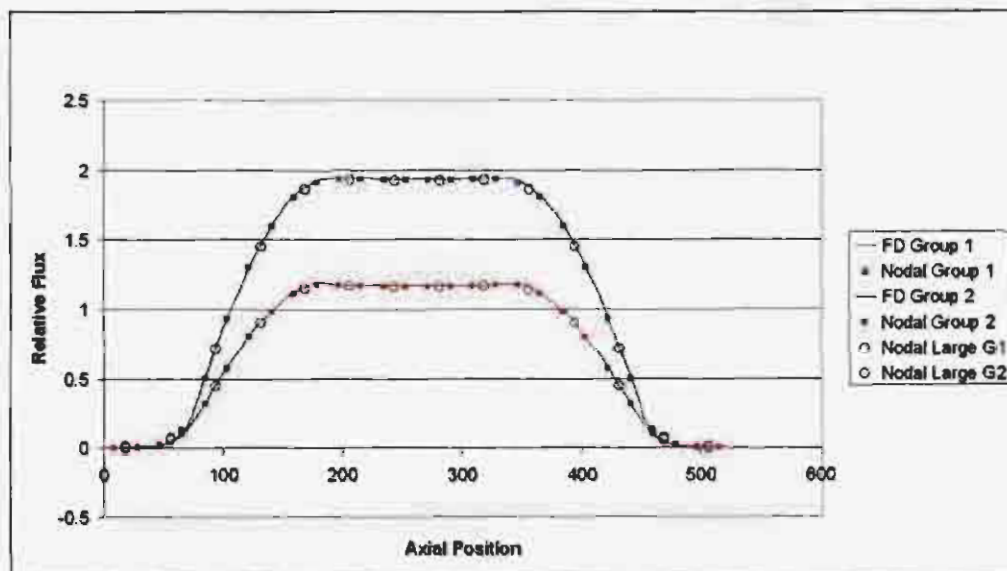


Figure 6.2: Dodds 2D (r, z) - axial profile (radially-averaged)

Figures 6.1 and 6.2 show good agreement with FD for both fast and thermal groups (groups 1 and 2 respectively), on both nodal meshing schemes. Since this problem is only a 2D construction and exhibits only mild flux gradients, a more detailed accuracy and performance evaluation of results is left for the subsequent PBMR and IAEA LWR model problems. We conclude this section by noting that, for the Dodds' benchmark problem, NoRTHZ shows excellent eigenvalue and flux agreement with fine-mesh finite-difference.

It may be interesting to note that, during the calculation of this problem and for some of those to come, numerical difficulties were often experienced near system boundaries during early nodal iterations. This is caused by inaccurate initial-guesses for the transverse leakage sources (which is the only source in these nodes in the fast group). These problems were handled by neglecting transverse leakage contributions in non-fuel zones in the early iterations (first couple of outers), but only for the nodes in which such problems are detected. This approach, although not rigorous in nature, works well and is implemented as a standard feature of the test code.

6.2 PBMR application

PBMR was identified as one of the primary application areas, and primary goals, of the work in this dissertation (see Section 1.5). The chosen problem for such an application is the 400

Two-dimensional description

Figure 6.3 separates broad material type regions by colour (reflector, core, rod, etc.) and areas of different cross-sections are indicated by the overlayed mesh. It is worth noting (from the figure) that the average radial mesh is in the order of 20 cm, while the diffusion length is in the order of 40 cm (this may be seen from the cross-sections for this problem listed in [17]). The implication hereof was touched upon in Section 1.2, where the statement was made that nodal methods reach their optimum performance when the mesh sizes (regions of constant

cross-section) are in the order of 5-8 diffusion lengths. The cross-section region sizes in this PBMR problem, which are in the order of a single diffusion length, could therefore limit the theoretical performance advantage which nodal methods may provide. This statement will be further investigated in the subsequent sections.

The problem is implemented as described in the benchmark specification, with one exception regarding the modeling of void regions. Void regions (indicated in the above figure) are modeled in the PBMR benchmark with zero removal cross-sections. Although this is not an inherent problem for the nodal method, special numerical expansions are required which are not yet implemented within the current test code. For the purpose of this comparison, the void region will be replaced with reflector material.

Three-dimensional description

The 3D problem description superimposes the (r, θ) layout in Figure 6.4 onto the (r, z) layout in Figure 6.3. Notice from Figure 6.4 that the only azimuthal inhomogeneity occurs in the vicinity of the control rods. Note further that this figure represents the (r, θ) cut of the roded region of the core only, with the "Rod" cross-sections replaced with reflector material everywhere below the level of the rod insertion.

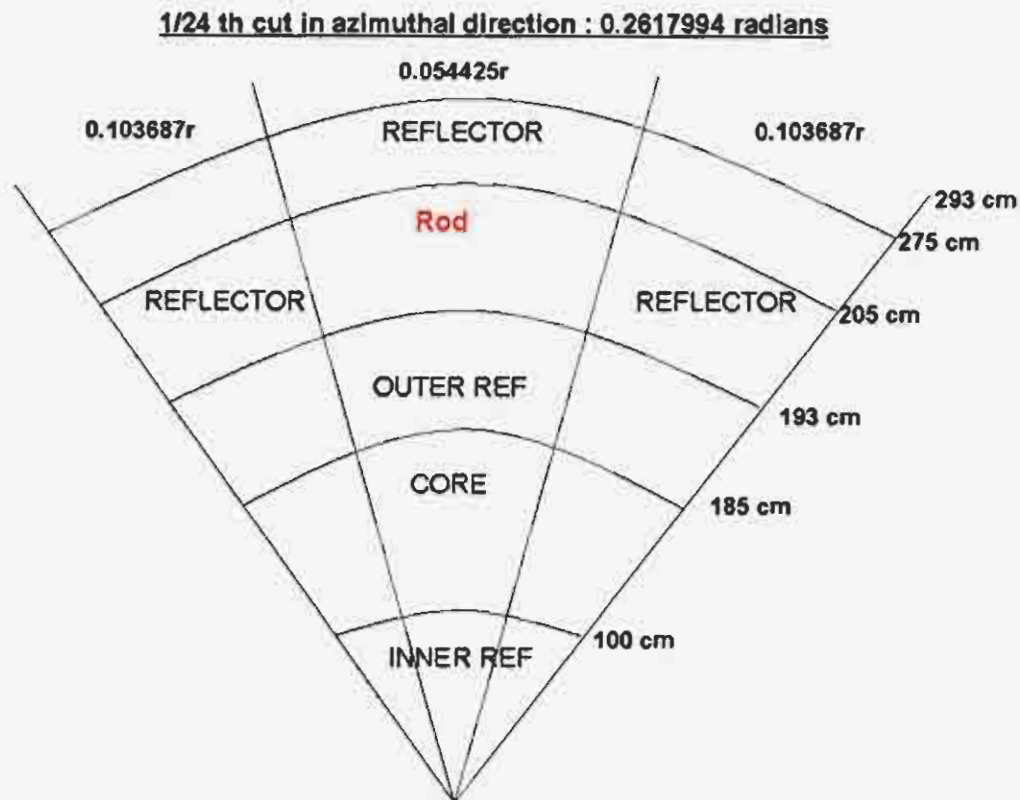


Figure 6.4: 3D PBMR 400 - (r, θ) projection (not to scale)

Two- and Three-dimensional models within SciFi and NoRTHZ

Both the 2D and 3D model results are presented for different refinement levels, for which certain terminology is defined here:

- *Coarse-mesh* - calculational mesh equal to the cross-section mesh in Figures 6.3 and 6.4.
- *2D FD reference mesh* - ten times refined radial mesh, five times refined axial mesh. This represents a converged finite-difference (FD) solution (10×5) .
- *3D FD reference mesh* - seven times refined radial mesh, twice refined axial mesh, three times refined azimuthal mesh. This represents a converged FD solution $(7 \times 2 \times 3)$.

Note that the presented 2D nodal calculation results are obtained utilizing the conformal mapping technique, making use of a single homogeneous azimuthal zone. The nodal calcu-

lations are carried out on the *Coarse-mesh*, with the exception of some radial refinement near the origin (three additional meshes). This is done to limit the magnitude of the "ghost" inhomogeneous source as was suggested in Section 5.3.

Two-dimensional results

Eigenvalue results from the 2D problem are presented, along respective calculational times, in Table 6.2.

Calculation	k-eff (error)	Time (min)
FD Reference	1.00046 (0 pcm)	70
<i>FD Coarse-Mesh</i>	0.99147 (898 pcm)	0.2
<i>Nodal (flat leakage)</i>	1.00079 (34 pcm)	3
Nodal (quad leakage)	1.00060 (14 pcm)	3.2

Table 6.2: 2D PBMR global results (nodal vs FD)

The comparative results indicate that the nodal approach provides much improved accuracy at a fraction of the calculational cost. Figure 6.5 further supports the quantification of this statement.

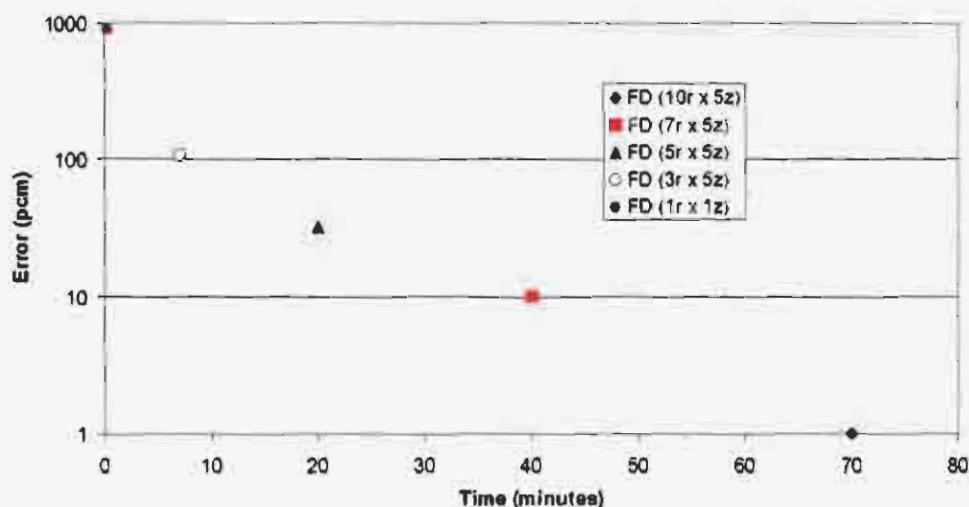


Figure 6.5: FD convergence error vs performance (calculational time)

In Figure 6.5 the finite-difference error vs. calculational time is tabulated for various refinement levels (error largely sensitive to refinement in the r -direction). From the data in the figure we deduce that a finite-difference calculation which produces nodal accuracy would take between 30 and 40 minutes (quadratic leakage nodal accuracy is 14 pcm). Since the running time for the nodal calculation was 3.2 minutes, we may deduce that for the PBMR (r, z) design, the nodal implementation provides an **approximate 2D performance advantage factor of 10 for equivalent finite-difference accuracy**. This is an important result, but conclusions and discussions concerning this result is left for later in this chapter.

As further illustration, Figures 6.6 and 6.7 below show the radially and axially-averaged flux profiles respectively, of the (r, z) problem for both the reference FD and nodal approaches. The figures illustrate both fast (group 1) and thermal (group 2) flux profiles, normalized to produce a full-core power level of 400 MW.

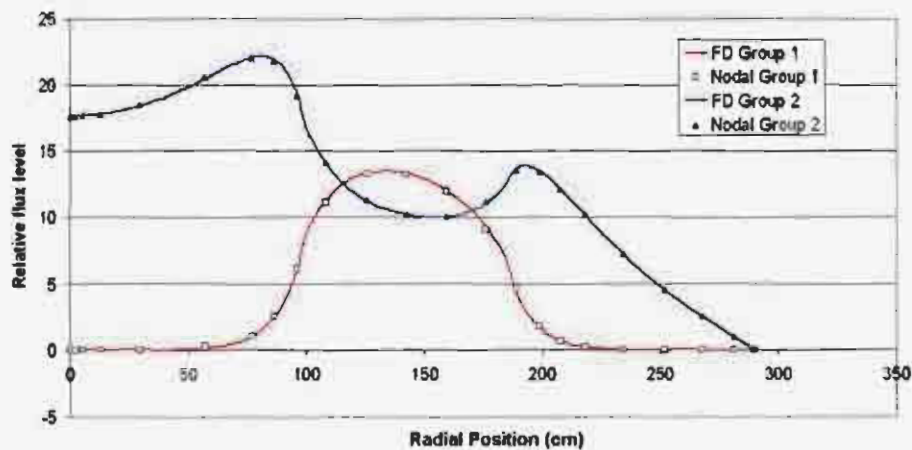


Figure 6.6: PBMR benchmark radial multi-group flux profiles (axially-averaged)

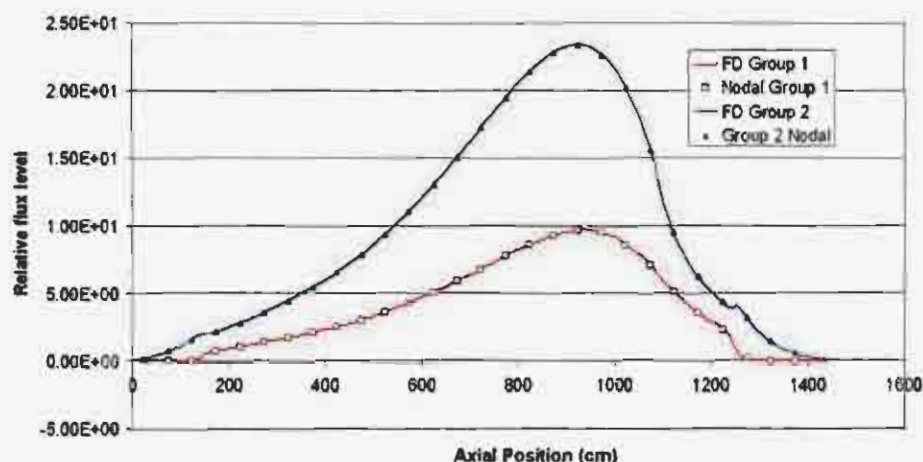


Figure 6.7: PBMR benchmark axial multi-group flux profiles (radially-averaged)

It is clear that there is a good match between the nodal and the reference finite-difference flux profiles. As discussed at the outset of this problem, the number of nodal meshes is not optimal, but this is a result of relatively small regions of constant cross-section throughout the benchmark configuration.

Figure 6.6 provides some insight as to why a radial 2.5 cm FD mesh is required on a reactor with an average 25 cm diffusion length. We notice that the reactor design causes relatively large flux gradients and this fact requires a finer discretization than would be otherwise expected (refer point 2 in Section 1.2).

We conclude that the 2D results indicate a definite nodal method advantage, although somewhat less than may typically be expected for this class of methods as applied to light water reactors. We will proceed to evaluate this advantage factor for a 3D calculation, in which case the conformal mapping technique is applied fully (inhomogeneities in both mapped directions).

Three-dimensional results

The results of the 3D calculations (performed with both the test codes) are presented in Table 6.3.

Calculation	k-eff (error)	Time (min)
FD Reference (extrapolated)	0.999682	-
FD Coarse-mesh	0.992558 (713 pcm)	1.6
FD Intermediate-mesh ($4 \times 2 \times 3$)	0.999275 (41 pcm)	190
Nodal (flat leakage)	1.000290 (61 pcm)	16.6
Nodal (quad leakage)	0.999562 (12 pcm)	15.5

Table 6.3: 3D PBMR global results (nodal vs FD)

Due to long calculational times, the reference FD solution was obtained via extrapolation from a series of finite-difference calculations. Figure 6.8 shows 3D finite-difference accuracy as a function of calculational time for various refinement levels.

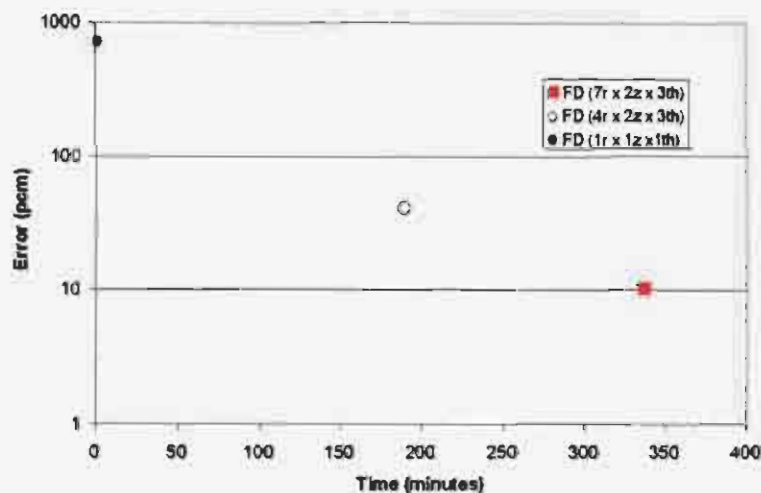


Figure 6.8: 3D FD convergence error vs performance (calculational time)

Utilizing Figure 6.8 and Table 6.3, and employing the same logic as in the 2D case, a reasonable estimate for the nodal advantage factor for a 3D PBMR reactor calculation is found to be in excess of 20. This is the major result from this chapter, and we claim that this developed nodal method allows for a significant performance increase for PBMR. Nevertheless, the factor 20 for PBMR is somewhat less than what could typically be expected from nodal methods for light water reactors (the order of a factor 100 is reasonable),

and this discrepancy could be attributed to the relatively small size of cross-section regions as compared to the diffusion length within PBMR. The reasoning behind the choice of cross-section region sizes for the published 400 MW PBMR benchmark [17] is outside the scope of this work.

The ability of the nodal code to reproduce all the flux features inherent to a real 3D PBMR problem is shown in Figure 6.9. The graph shows two azimuthally different radial thermal (group 2) flux profiles, axially through the center of the first roded (containing a control rod) mesh. *Zone 1* represents the azimuthal reflector region adjacent to the control rod mesh, and *Zone 2* represents the radial profile through the control region itself.

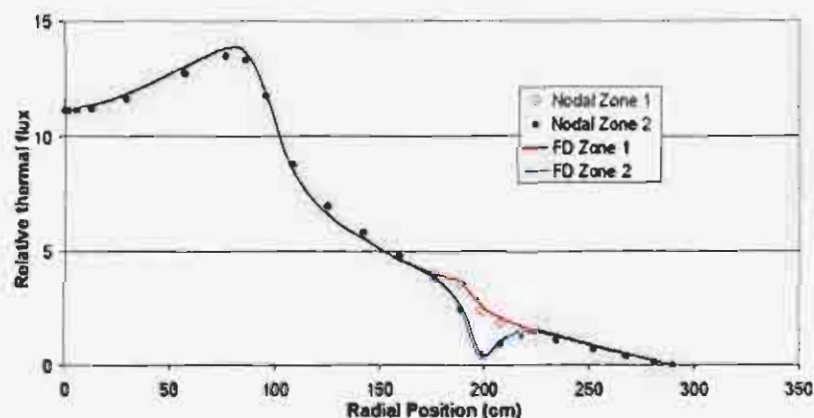


Figure 6.9: PBMR: Radial profile through and adjacent to control

It is interesting to note that, for the benchmark equilibrium operating state, the azimuthal dependency, which exists only in the control rod region, causes a localized azimuthal flux perturbation. This may imply that many calculational meshes are unnecessary and highlights the possible need for a non-standard azimuthal discretization (varying azimuthal refinement for different radial zones).

Figure 6.10, in conclusion, presents the azimuthal group flux profiles through the radial zone containing the control rod (see Figure 6.4) and axially at the level of the rod tip.

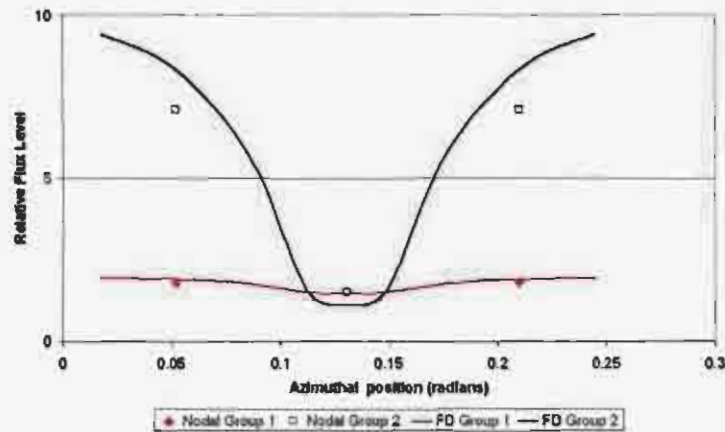


Figure 6.10: PBMR: Group fluxes through control - azimuthal profile

Figure 6.10 once again reveals good general agreement, remembering that the nodal results are averages for material regions. From Figures 6.9 and 6.10 we may conclude that the control rod region still acts largely as a 2D control blanket. This allows the practical use of 2D calculations for many typical PBMR core calculations.

Concluding remarks

The PBMR design, as depicted in this section, is seen as the intended application area of this work, and the successful application of the approach to the published benchmark signifies one of the major goals of this thesis. Nevertheless, in order to test the method fully, and to develop some future work areas, the conformal mapping approach, in the next section, is applied to a much more difficult neutronic problem than represented by the PBMR design. This problem will also conclude the results and discussion chapter.

6.3 IAEA cylindrical 3D benchmark

The final numerical problem addressed in this thesis, is a "cylindrisized" version of the 3D IAEA PWR benchmark problem described in [7]. For the sake of this work, the benchmark has been adapted to cylindrical coordinates by closely matching the volumes of fuel, control and reflector material, and hence preserving the nature of the flux gradients in the problem. This problem should test the conformal mapping approach thoroughly, since it exhibits severe material inhomogeneities in all three dimensions. The detailed description of the

constructed problem may be found in Appendix D. As basic illustration, Figures 6.11, 6.12 and 6.13 describe the general material layout.

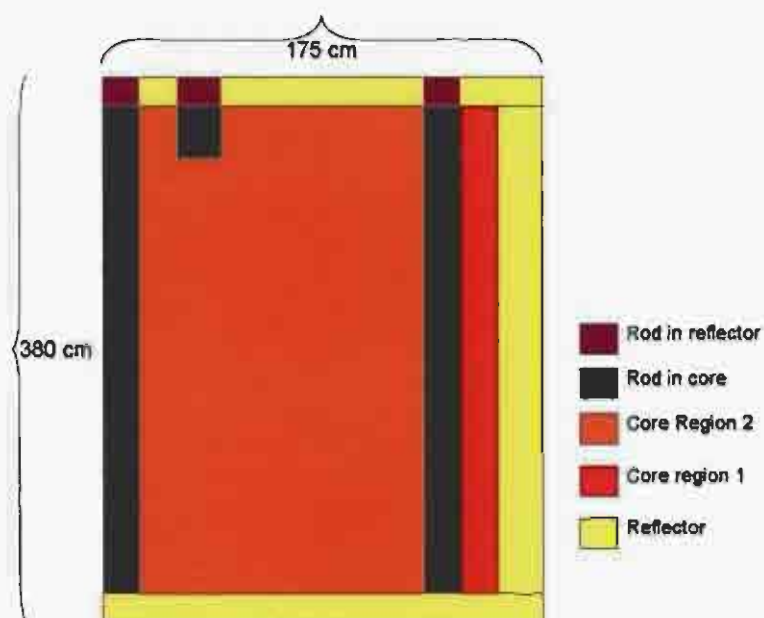


Figure 6.11: IAEA (r, z) layout - azimuthal cut at 45 degrees

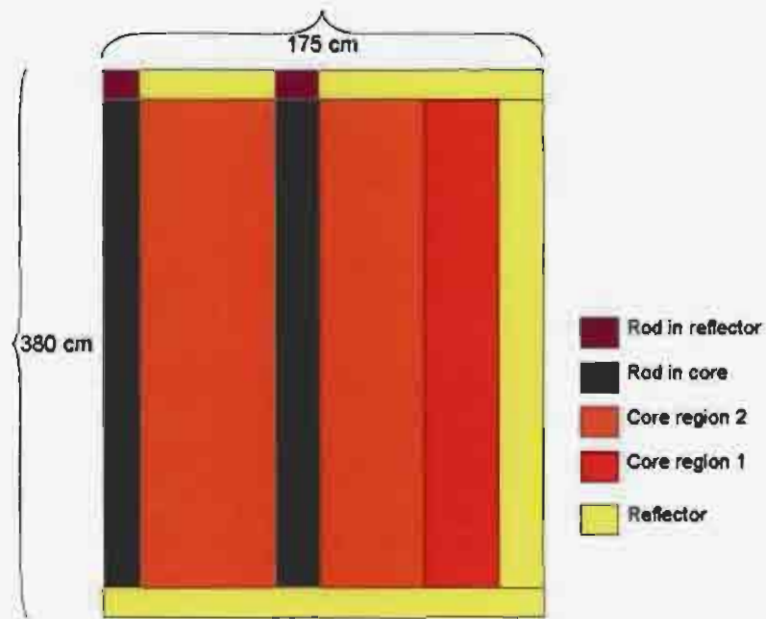


Figure 6.12: IAEA (r, z) layout - azimuthal cut at 0 degrees

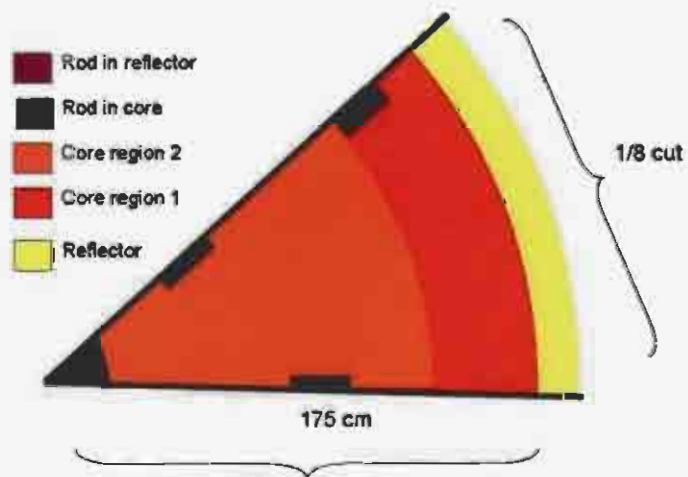


Figure 6.13: IAEA (r, θ) layout - top view

The aim of applying the NoRTHZ code to this problem is two-fold:

- Evaluate the accuracy of the method for such a severely inhomogeneous neutronic design.
- Identify deficiencies in the proposed method and define future improvements.

Global results

Eigenvalue calculations were performed with both SciFi and NoRTHZ for the above configuration, and global results are listed in Table 6.4. The nodal calculation was performed upon a mesh with average axial- and radial sizes of approximately 20 cm, and the finite-difference refinement factors upon this mesh are listed in Table 6.4. The final two columns, named "RZ" and "R θ ", list the maximum and the average power error from two perspectives. The "RZ"-column gives the (average and maximum) azimuthally-averaged (r, z) errors, and the "R θ "-column gives the (average and maximum) axially-averaged (r, θ) errors. "R θ " may be interpreted as the traditional assembly averaged powers for each axial channel. These definitions are introduced in order to represent a very large number of results as concisely as possible. The average and maximum power errors reported in the table are for fuel regions in the system and the power in any node n is given by $P_n = \sum_{g=1}^G w^g \sigma_{f,n}^g \Phi_n^g$ where w^g represents the energy released per fission. The mesh on which these results are generated is described in Appendix D.

Method (RxZxTh)	k_{eff}	Time	k_{eff} Error	RZ(Ave,Max)	R θ (Ave,Max)
Extrapolated	1.02420	—	—	—	—
FD(12x12x12)	1.02410	34378 min	10 pcm	1% (3%)	1% (1.7%)
FD (8x8x8)	1.02399	6202 min	21 pcm	2% (6.2%)	2% (3.5%)
FD (6x6x6)	1.02388	2105 min	31 pcm	3% (9.4%)	3% (5.4%)
FD (4x4x4)	1.02378	242 min	41 pcm	4.8% (15%)	4.6% (8.7%)
FD (2x2x2)	1.02468	7.2 min	47 pcm	6.5% (20.2%)	5.6% (12.5%)
FD (1x1x1)	1.02985	0.1 min	552 pcm	6.1% (29.6%)	6.6% (22.1%)
Nodal - flat leakage	1.02483	9.2 min	62 pcm	0.84% (5.4%)	0.8% (2.6%)
Nodal - quad leakage	1.02424	10.2 min	4 pcm	0.5% (6.9%)	0.5% (2.8%)

Table 6.4: Eigenvalue results for 3D IAEA benchmark problem

The reference flux results were obtained via extrapolation using results from the $(6 \times 6 \times 6)$, $(8 \times 8 \times 8)$ and $(12 \times 12 \times 12)$ finite-difference calculations as listed in Table 6.4. An extrapolated solution was also obtained for the system eigenvalue (k_{eff}). This extrapolation function, utilizing results from the same refinement levels as for the flux, and assuming a quadratic approach to convergence, is found to be

$$y = 0.001x^2 - 0.0013x + 1.02420$$

and is plotted in in Figure 6.14. From this function the extrapolated value for k_{eff} is found for a 0 "Weighted refinement factor" and has a value of 1.02420. This approach is consistent with the procedure followed in [7] for the Cartesian equivalent of this problem, and is not further described here.

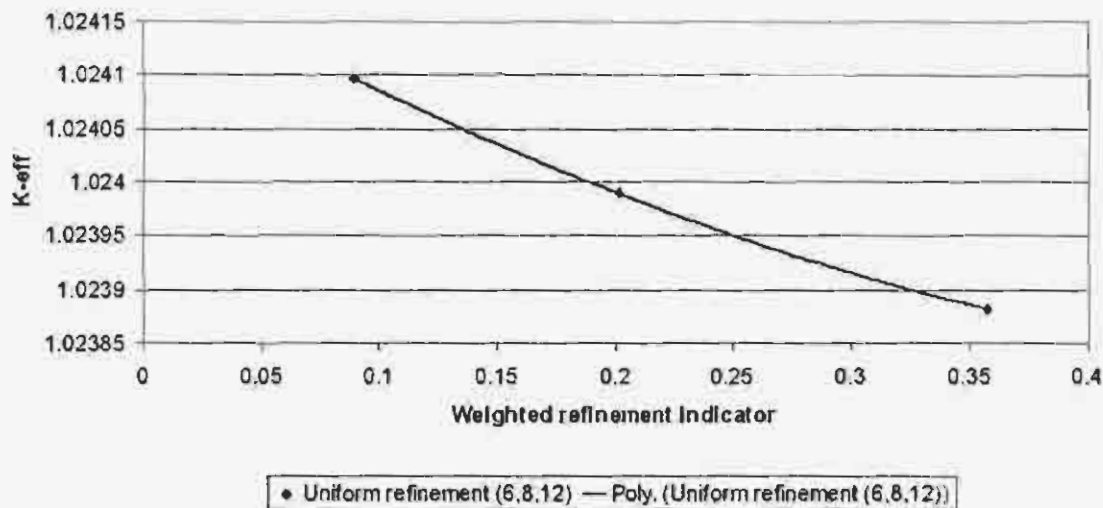


Figure 6.14: IAEA eigenvalue extrapolation - 2nd order fit for uniform refinement

Firstly we notice, from Table 6.4, that the nodal solution is extremely accurate in eigenvalue (within 4 pcm of the extrapolated result). We may further utilize Table 6.4 to estimate the performance advantage factor for the proposed nodal method over finite-difference results. We notice a much larger improvement in relative calculational time as compared to the PBMR in the previous section and an estimation of the performance advantage factor

over a finite-difference calculation of equivalent accuracy may once again be performed. Inspection of Table 6.4 shows that the $(8 \times 8 \times 8)$ finite-difference calculation is approximately equivalent in accuracy to the nodal calculation with quadratic leakage (considering both k_{eff} and powers).

We therefore deduce, by considering the relative calculational times of these two calculations, that **the performance advantage factor of nodal over finite-difference is well in excess of 500**. In the case of the IAEA benchmark problem, flux gradients are large in all three dimensions, and are coupled with a much smaller neutron mean free path (order of 1 cm). These factors cause that, for the IAEA problem, the nodal method provides a much larger performance advantage factor than for PBMR. As expected, the inclusion of the quadratic leakage approximation significantly improves the eigenvalue for this problem.

We further note from Table 6.4, that the maximum nodal (r, z) power error is 6.9%, and maximum nodal (r, θ) error is 2.8%. These discrepancies require further attention and are investigated in the next section.

Flux profile comparisons

In order to investigate the nature of the averaged nodal power errors, Figures 6.15 and 6.16 illustrate errors in the thermal flux within the core. Nodal flux errors, as compared to extrapolated finite-difference, are presented firstly as an (r, z) contour plot and secondly as an (r, θ) contour plot (the contour plots are given for both flat and quadratic leakage approximations). Once again (r, z) results are azimuthally-averaged and (r, θ) results are axially-averaged.

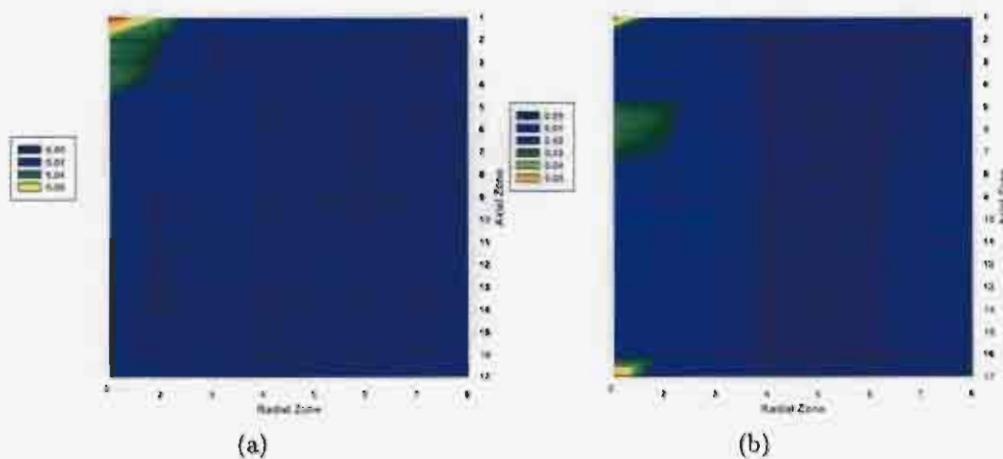


Figure 6.15: IAEA (r, z) thermal flux errors - (a) quadratic leakage (b) flat leakage

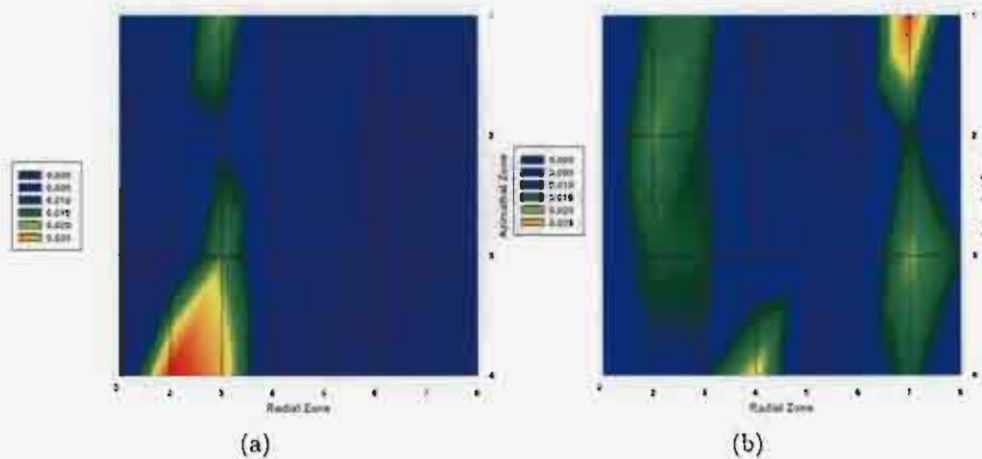


Figure 6.16: IAEA (r, θ) thermal flux errors - (a) quadratic leakage (b) flat leakage

From the above results, the following may be deduced:

- The maximum flux errors (6% for the (r, z) case, 2.5% for the (r, θ) case) occur near the radial center of the system, and in the axial top of the model.
- It is visible that the quadratic leakage cases in (a) of both Figures 6.15 and 6.16 show larger maximum errors, but in isolated positions. The flat leakage approximation in (b) shows lower maximum errors, but a broader distribution of error throughout the system, and hence a less accurate eigenvalue (see Table 6.4).

To provide some perspective on these errors, Figure 6.17 is presented and shows the reference flux profiles for both the azimuthally-averaged (r, z) and axially-averaged (r, θ) plots.

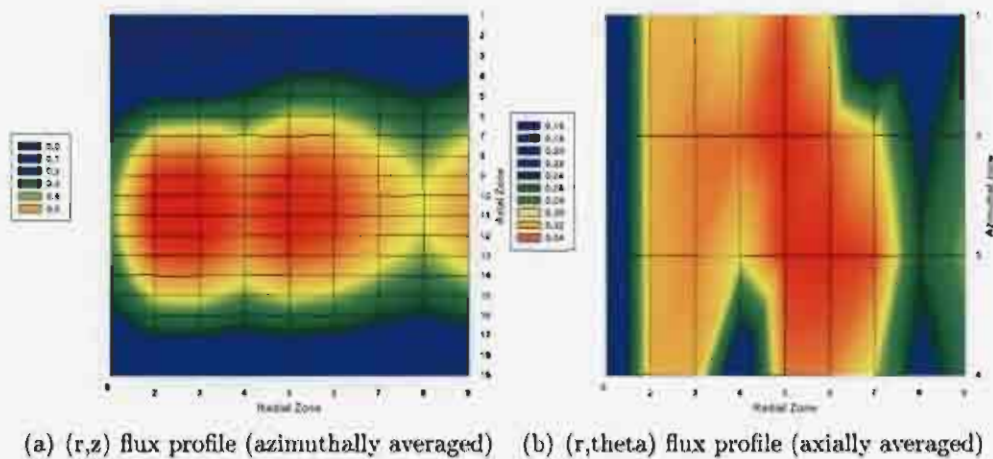


Figure 6.17: IAEA thermal profiles

From the above, we notice that the errors in Figures 6.15 and 6.16 occur in relatively low flux regions of the core (especially the larger (r,z) errors), and thus diminishes the importance of these larger relative errors. Nevertheless, these errors are larger than would normally be expected from nodal methods and possible causes for these errors are now discussed.

Inner cut-out approximation

Figure 6.18 illustrates the radial thermal flux profile through the axial top of the model, and supplies some insight into a further possible reason for the inner flux error.

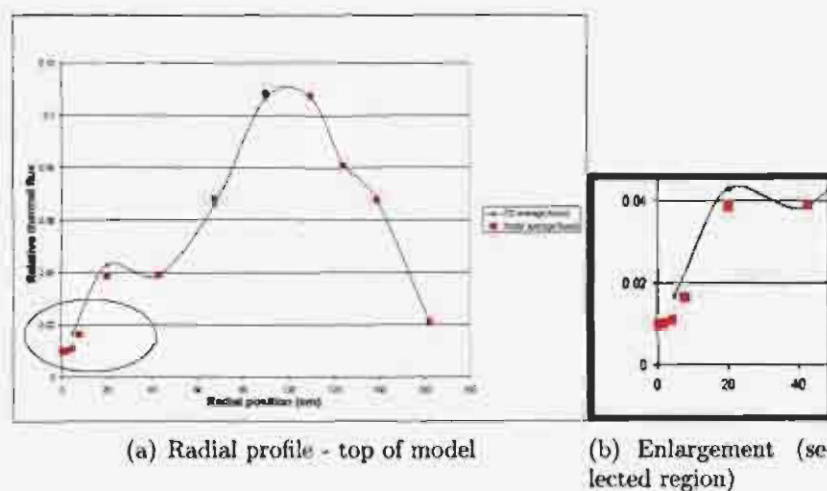


Figure 6.18: IAEA radial thermal profile through axial top of core

In Figure 6.18 the adherence of the nodal solution to the inner boundary condition at 1 cm is visible, but does not signify a physical characteristic of the flux solution. In the previous section, the PBMR model did not exhibit this problem, since the flux solution was near constant in the center of the system. Furthermore, this effect is compounded by the use of the quadratic leakage approximation near the center, since this approach makes use of a three node fit to approximate the transverse leakage terms. The error therefore propagates some distance into the system. This result highlights the need to include the inner zone within the solution process, even if this is done in an approximate manner.

Some future suggestions in this regard include:

1. A hybrid leakage approximation, making use of the flat approximation near the center, and the quadratic approximation throughout the rest of the system. This approach would avoid using the inner zone in leakage approximations near the center.
2. A hybrid finite-difference / nodal solution in the center of the system. Such an approach would make use of the fact the the central cut-out region is small (in the order of 1 cm for the sake of current implementation), and therefore do not require many finite-difference meshes to reproduce a reasonable result. Thus, such a solution would not significantly affect the performance.
3. A representative energy dependent albedo boundary condition at the edge of the cut-out, updated during the calculational procedure. Such an update may be based upon the intra-nodal solution within the neighbouring mesh.
4. A rigorous analytic solution for the inner homogeneous disc. Such an approach would be more accurate, but may incur complexity not justified by the improvement.

Inner radial quadratic leakage contamination

These prior four additions fall, in general, outside the scope of the current thesis. Nevertheless, point 1 above has been implemented into the test code and is termed the **mixed leakage approximation**. This approach entails using the flat (single node) transverse leakage approximation within the first few radial meshes, and thereafter apply the quadratic leakage approximation to the rest of the system. The motivation lies therein that the error caused by the inner cut-out should not be allowed to propagate into the rest of the system. Global results are presented in Table 6.5 and contour plots in Figure 6.19 ((r, z) and (r, θ)).

Method	Eigenvalue	Time	k Error	RZ(Ave,Max)	R θ (Ave,Max)
Extrapolated	1.02420	—	—	—	—
Nodal - flat leakage	1.02483	9.2 min	62 pcm	0.84% (5.4%)	0.8% (2.6%)
Nodal - quad leakage	1.02424	10.2 min	4 pcm	0.5% (6.9%)	0.5% (2.8%)
Nodal (mixed leakage)	1.02436	10 min	15 pcm	0.4% (6.5%)	0.4% (1%)

Table 6.5: Eigenvalue results for IAEA benchmark - mixed leakage approximation

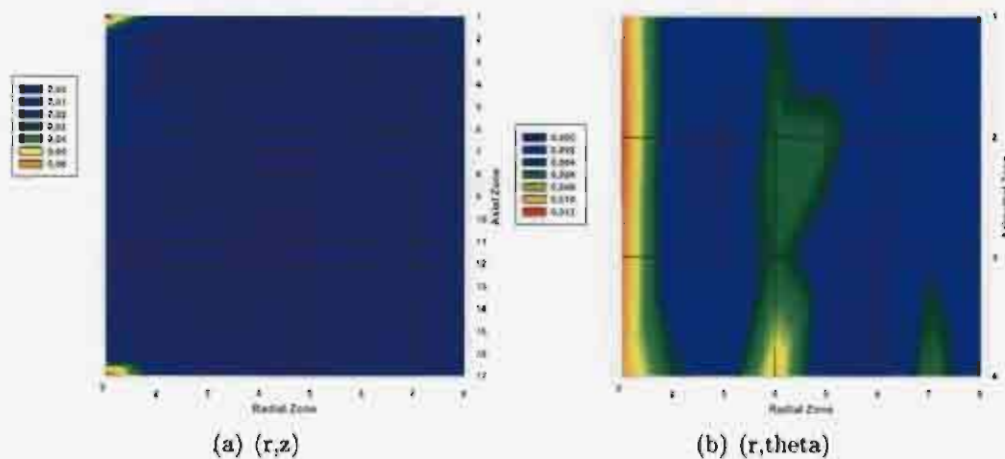


Figure 6.19: IAEA thermal flux errors for the mixed leakage approximation

Table 6.5 shows a slight degradation in k_{eff} by using the mixed approximation, but a dramatic improvement in the (r, θ) plane maximum error from 2.8% to 1%. A general improvement in error distribution is also visible by comparing Figure 6.19 with Figures 6.15 and 6.16. Although this mixed leakage approach does improve results for this problem, the argument for its use is largely intuitive, and should be investigated further. The radial position chosen for the change from flat to quadratic leakage was about one third into the system. Note that the flat leakage approximation is only applied in the radial direction, and that the one-dimensional equations in both azimuthal and axial directions still utilize the quadratic leakage approximation throughout the system.

This approach resolves the discrepancy in the (r, θ) plane, but the error in the (r, z) plot improves only marginally. This can be seen from Table 6.5, where only a slight improvement from 6.9% to 6.5% in the RZ maximum error occurs.

Nodal aspect ratios

The quadratic leakage approximation provides important improvements in results, and specifically in cases where nodal aspect ratios (measure of nodal skewness) are not excessively large (typically less than a factor of 10). Figure 6.20 indicates nodal aspect ratios for the system. Note that, since all axial zones are 20 cm in size, the $z : r$ and $z : \theta$ aspect ratios need only be given for a single (r, θ) plane.

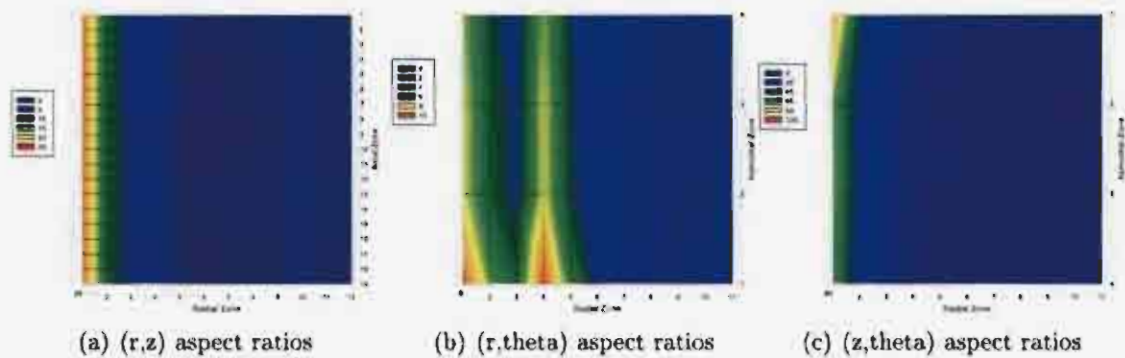


Figure 6.20: IAEA nodal aspect ratios

From Figure 6.20 it is clear that a wide range of aspect ratios exist, with many directional ratios exceeding typical aspect ratios for quadratic leakage. This occurs mostly near the center of the cylindrical system. Values which are especially large occur in the $z : \theta$ ratio near the center of the system and may be a contributing factor to the central errors. Solutions to this situation are largely problem dependent, but become more prevalent in systems with central inhomogeneity. Here, once again, the coupled finite-difference/nodal hybrid is suggested as a future extension in order to lessen the dependence on the quadratic leakage approximation near the center of the system, particularly in situations where a flat leakage approximation is not sufficiently accurate.

Concluding remarks

The application of the proposed method to the cylindrisized version of the IAEA benchmark problem has provided valuable insight into both the advantages and shortcomings of the method. This problem signifies a computationally and neutronically difficult problem, and the accuracy achieved by NORTHZ proves that the method works (4 pcm error in eigenvalue) and provides a substantial performance improvement (factor in excess of 500). On the other

hand, the benchmark problem is also sufficiently difficult to highlight some shortcomings of the approach, specifically associated with the center cut-out approximation and the usage of the quadratic leakage approximation in this area. These factors lead to larger flux errors on the periphery of the system. In these low flux areas, care must also be taken to implement appropriate Taylor series expansions to eliminate possible round-off errors, specifically in the calculation of higher order flux moments. These expansions are considered an important future addition to the solution method as well as a coupled finite-difference/nodal solution for the inner disc. A more consistently defined hybrid of the flat and quadratic leakage approximation is also foreseen, since this approach reduced errors in axially integrated powers to within acceptable levels for nodal methods.

Final remarks regarding results

Three problems were investigated in this chapter, all of which relate to published benchmark problems. The problems represent various degrees of difficulty, and the NoRTHZ code performed well in all cases. It may be concluded that the needed assumptions in the development, such as (a) the inner cut-out approximation (Section 3.3) (b) the variable separation for the one-dimensional azimuthal source terms (Section 3.4.2), and (c) the fourth order polynomial approximation to the inhomogeneous geometric sources (Section 5.2), are numerically justified in both accuracy and performance, although some small outstanding issues remain. The final chapter now follows, and gives general conclusions concerning the entire scope of this dissertation as well as potential future work.

Chapter 7

CONCLUSIONS AND FUTURE WORK

7.1 Introduction

The development, test implementation and verification of the conformal mapping approach to the analytic nodal method, as described in this dissertation, signify some progress in the field of method and code development for HTR reactors. The decision regarding the usage of this method in daily PBMR design calculations is still under discussion, but results in this thesis will go some way in supporting that objective. This chapter serves to summarize the major conclusions gathered during the development of this work and supplies, at a glance, the advantages and shortcomings of this approach. The development of this work has lead to four international, refereed conference publications, received an award for best paper by a young researcher, and has been nominated for publication in the Nuclear Engineering and Design journal (submission in March 2007). These publications are listed below:

1. Rian H. Prinsloo, Djordje I. Tomašević, "Development of the Analytic Nodal Method in Cylindrical Geometry", Proceedings of Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Application 2005, Avignon, France, September 2005 on CD (2005).
2. Rian H. Prinsloo, et al., "Application of SP2 and the Spatially Continuously SP2-P1 Equations to the PBMR reactor ", Proceedings of Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Application 2005 , Avignon, France, September 2005 on CD (2005).
3. Rian H. Prinsloo, Djordje I. Tomašević, "Development of the Analytic Nodal Method

in Cylindrical Geometry for PBMR Application", 3rd International Topical Meeting on High Temperature Reactor Technology (HTR 2006), Johannesburg, South Africa, October 2006 on CD (2006).

4. Rian H. Prinsloo, Djordje I. Tomašević, "Approach to Singular Regions in the Conformally Mapped Analytic Nodal Method in Cylindrical Geometry", Submitted and accepted for publication at Mathematics and Computation, Supercomputing, Reactor Physics and Nuclear and Biological Application 2007, Monterey, California, USA, April 2007 on CD (2007).

The major stepping stones of this work are discussed throughout these publications. In the following section, a more global perspective upon the work, its conclusions, relevant contributions and future work are presented.

7.2 General conclusions

1. Day-to-day design calculations for the South African PBMR reactor are largely performed with legacy code systems, and many advances in the field of method and code development have not been incorporated into these systems. One such improvement relates to the use of nodal methods for the sake of full core neutronic, diffusion solutions.
2. The diffusion equation in cylindrical geometry poses problems during transverse integration within the Analytic Nodal Method. A proposed solution to circumvent these difficulties is to apply conformal mapping, to locally map a node in cylindrical coordinates into a rectangular one, and then apply transverse integration in Cartesian coordinates. The important node-averaged flux to surface-averaged current relationship is obtained in mapped coordinates and finally mapped back to original cylindrical coordinates for insertion into the balance equation. Care must however be taken in the polynomial order of the approximation of the exponential mapping function. This development is described in Chapter 3.
3. The equations derived in Chapter 3, based on the conformal mapping approach, are practical and manageable, both for the sake of implementation and efficiency. The final equations are similar in nature to nodal methods with intra-node residual sources (e.g. intra-node cross-section feedback), and were successfully implemented in a standalone FORTRAN code for numerical evaluation of the approach. A FORTRAN based

finite-difference solver, based upon the methodology described in Chapter 2, was also developed to serve as a reference solution generator for the nodal test code.

4. As shown in Chapter 4, the derived equations exhibit a fine-mesh limit, which is an important characteristic for the stability and accuracy of the method. Due to the nature of the conformal mapping approach, the derived fine-mesh limit is not valid in the center of the system.
5. Comparison with finite-difference results in Chapter 6 strongly supports the view that, for the first time, successful transverse integration has indeed been achieved via conformal mapping. Detailed flux profiles and global values of reactivity, for a variety of test problems, show that the implemented conformal mapping technique works as expected. Accuracy in eigenvalue, for the chosen set of test problems, is consistently at the order of 10 pcm as compared to reference finite-difference solutions.
6. For the first time, as far as the author was aware at the time of writing, the quadratic leakage approximation has successfully been applied to the ANM in cylindrical geometry. This addition provides a marked improvement in the quality of results for multidimensional problems, and based on the results in Chapter 6, may be seen as a necessity for practical reactor calculations.
7. It was shown in Chapter 6 that, although limited by PBMR design factors, the ANM still provides a 3D performance advantage factor of the order of 20 for a given accuracy, when compared to a finite-difference approach. In the case of a more typical LWR reactor, as in the case of the IAEA benchmark problem, the performance advantage factor is well in excess of 500.
8. As is visible from both Chapters 4 and 5, the conformal mapping approach does induce a mild singularity in the center of the system, and this may be seen as a shortcoming of the method. Due to this, a homogeneous cut-out is necessary in the center, making use of some form of coupled auxiliary solutions for the cut-out region. A further impact of the approach relates to some meshing restrictions near the center of the system, requiring typically two or three more nodal meshes near the center than some material distributions would require.
9. The inner cut-out approximation does not pose any difficulties for the PBMR reactor design, but will need an improved formulation in the case of larger central inhomogeneity. The imposed zero net current boundary condition placed at the edge of the cut-out disc distorts the quadratic leakage approximation in cases where the flux profile near

the center is not constant. In such cases hybrid solutions between flat and quadratic leakage, and/or a coupled finite-difference/nodal solutions may provide substantial improvements. These issues were discussed and shown in Section 6.3.

10. All the above considered, nodal methods in general, and the developed conformal mapping approach to the Analytic Nodal Method in particular, certainly have a place in the arena of PBMR core calculational methods. Some improvements may still be required for the method to become fully practical for day-to-day calculations, and some of these identified requirements are listed in the next section.

7.3 Future work

During the development of this work, further developments outside the scope of the thesis were identified as natural next steps. These are:

1. The method will be implemented in the Ncsa developed OSCAR code system [22], which utilizes standard acceleration schemes. This will allow realistic calculational times (improvement by approximately a factor of 20) to be obtained, and support decisions to be made regarding the inclusion of the method in PBMR calculational schemes.
2. Improved methods for the solution of the homogeneous central disc, and potentially for the solution of an azimuthally inhomogeneous central disc.
3. Taylor series expansions for small arguments are required in the case of flux moment calculations. These are of specific use in problems with large reflector nodes where the flux reaches relatively low levels near system boundaries. Furthermore, such expansions would allow increased flexibility, such as the calculation of void regions needed in Section 6.2.
4. The PBMR design raises interesting potential improvement needs within the nodal formalism, such as intra-node homogenization techniques to maximize the nodal performance advantage, and non-standard or variable azimuthal discretizations applied to localized azimuthal dependencies.

7.4 Final considerations

The successful integration of the proposed method into an industrial code system will require further testing, development, verification and validation. Furthermore, the optimal applica-

tion of the method will require new methods, and adaptation of existing ones, in other areas of the reactor calculational path. These adjustments and extensions will take some time and focused effort. Nevertheless, this work provides a solid foundation for further development.

Other nodal solution methods, many of which were mentioned in the opening chapter, may provide the final solution to the PBMR core diffusion problem. Decision makers in this regard will make these choices at the appropriate time, but in the very least the South African developed **Cylindrical Analytic Nodal Method** has now been added to this list.

Appendix A

TEST CODE USER MANUAL

The input manuals for both SciFi and NoRTHZ are very similar, and hence, as illustration, only the SciFi input manual is fully described in this appendix.

SciFi user manual

SciFi input is CARD type, with each card preceded with a compulsory comment field. The data specification is free format and follows below. When multiple entrees are required per line, the description will be separated by a semicolon.

Version Card

- COMMENT: STRING [255]
- VERSION: STRING [255]

Example input:

- '* COMMENT'
- 'SciFi V1.00'

Title Card

- COMMENT: STRING [255]
- TITLE: STRING [255]

Example input:

- '* COMMENT'
- 'TEST Problem 1'

Date Card

- COMMENT: STRING [255]
- DATE: STRING [255]

Example input:

- '* COMMENT'
- '04/05/2004'

Description Card

- COMMENT: STRING [255]
- DESCRIPTION: STRING [255]

Example input:

- '* COMMENT'
- 'This problem is run as an input test'

Output file name Card

- COMMENT: STRING [255]
- OUTPUT FILENAME: STRING [255]

Example input:

- '* COMMENT'
- 'OUTPUT.PRT'

Iteration Card

- COMMENT: STRING [255]
- Max outer iterations: INT; Max inner iterations: INT; Relaxation parameter: REAL(8); Flux convergence criteria: REAL(8); Power Normalization Factor: real(8); DEBUG PRINT-OUT: INT; SP2 calculation:INT; SP2-P1 parameter:REAL(8)

Example input:

- '* COMMENT'
- 200 400 1.3 0.0000001 1000000 2 0 0

Notes:

When the debug option ≤ 0 , only standard output is written to the output file, when greater to 1, incrementally more debugging information is written to the output file.

Energy Group Card

- COMMENT: STRING [255]
- Number of Groups: INT ; First thermal group: INT

Example input:

- '* COMMENT'
- 2 2

Notes

All thermal groups are automatically used in upscatter calculations. (if the cross-sections allow)

Fission Spectra Card

- COMMENT: STRING [255]
- Fission neutron fragment per group for (1 .. NUM_GROUPS): real(8) ;

Example input:

- '* COMMENT'
- 1.0 0.0

Calculational Mesh discretization Card

- COMMENT: STRING [255]
- Number of calculational Radial meshes: INT ; Axial: INT ; Azimuthal: INT

Example input:

- '* COMMENT'
- 40 40 4

Calculational Mesh Refinement Card

- COMMENT: STRING [255]
- Mesh refinement factor: Radial: INT ; Axial: INT; Azimuthal: INT

Example input:

- '* COMMENT'
- 2 2 2

Outer Radial boundary condition

- COMMENT: STRING [255]
- ALBEDO Value(1..G): real(8)

Example input:

- '* COMMENT - albedo for two group problem'
- 1.0 1.0

Notes:

An Albedo value of 1 indicates reflective boundary conditions, 0 indicates Zero Incoming Current, and -1.0 is used for Zero-flux condition. Any value between 0 and 1 may be used for specific albedo value.

Bottom axial boundary condition

- COMMENT: STRING [255]
- ALBEDO Value(1..G): real(8)

Example input:

- '* COMMENT'
- 0.0

Notes:

An Albedo value of 1 indicates reflective boundary conditions, 0 indicates Zero Incoming Current, and -1.0 is used for Zero-flux condition. Any value between 0 and 1 may be used for specific albedo value.

Top axial boundary condition

- COMMENT: STRING [255]
- ALBEDO Value(1..G): real(8);

Example input:

- '* COMMENT - albedo for two group problem'
- -1.0 -1.0

Notes:

An Albedo value of 1 indicates reflective boundary conditions, 0 indicates Zero Incoming Current, and -1.0 is used for Zero-flux condition. Any value between 0 and 1 may be used for specific albedo value.

Mesh and Source options

- COMMENT: STRING [255]
- MESH OPTION: INT ; FIXED SOURCE FLAG: INT

Example input:

- '* COMMENT'

- 1 0

Notes:

MESH OPTION = 0 indicates explicit mesh division input in card 14, MESH OPTION=1 indicates uniform, equi-distant mesh distribution defined in card 15, and MESH OPTION=2 indicates equi-volume remeshing described in card 16.

The FIXED SOURCE FLAG indicates the presence of fixed sources in some mesh regions, and will be described in CARD 21

Explicit mesh definition (only given if MESH OPTION = 0)

- COMMENT: STRING [255]
- Radial Mesh Sizes (1..Radial Meshes): real(8)
- Axial Mesh Sizes(1..Axial Meshes): real(8)
- Azimuthal Mesh Sizes (1..Azimuthal Meshes): real(8)

Example input:

- '* COMMENT'
- 2.0 3.0 3.0 4.0 4.0
- 1.0 1.0 1.0 2.0 2.0
- 1.571 1.571 1.571 1.571

Uniform (equi-distant) mesh definition (only given if MESH OPTION = 1)

- COMMENT: STRING [255]
- Radial Mesh Size: real(8) ; Axial Mesh Size: real(8)

Example input:

- '* COMMENT'
- 1.0 1.0 1.571

Equi-Volume mesh definition (only given if MESH OPTION = 2)

- COMMENT: STRING [255]
- Default Radial Mesh Size: real(8) ; Default Axial Mesh Size: real(8)
- Number of Coarse Radial Regions to Remesh: INT
- Boundaries for coarse regions(1..Num_regions+1): INT;

Example input:

- '* COMMENT'
- 8.0D0 18.75D0
- 5
- 1 6 16 21 27 33

Notes:

MESH OPTION = 2 requires an initial default mesh size to provide a reference for coarse-mesh boundaries. The coarse mesh regions will be remeshed within their boundaries specified in this card according to an equi-volume radial condition. (the total number of meshes will remain constant).

Material specification options

- COMMENT: STRING [255]
- Number of Materials: INT ; Material specification method (MSM) - 0 or 1: INT

Example input:

- '* COMMENT'
- 9 1

Notes:

Material Specification method(MSM) = 0 indicates explicit material identification for each radial, axial and azimuthal zone and is described in CARD 18 below. MSM=1 indicates combinational material placement, allowing for simultaneous assignment of a material to multiple indices and is described in CARD 19 below.

Explicit Material assignment (only given if MSM=0)

- COMMENT: STRING [255]
- MATERIAL ID NUMBER (1..ZMax,1..RMax,1..ArcMax): INT

Example input:

- '* COMMENT'
- 1 1 1
- 1 1 1
- 1 1 1
- 2 2 2
- 2 2 2
- 3 3 3

Notes:

The above input describes a 2 axial layer cylinder with 3 radial zones and 3 azimuthal zones. Material 1 is placed everywhere in axial zone 1, material 2 everywhere in axial zone 2, except the outer radial zone has material 3 in all azimuthal zones.

Combinational Material assignment (only given if MSM=1)

- COMMENT: STRING [255]
- *The following record is given until all axial zones are filled:*
- Zone name: STRING[255]
- Number of axial zones filled by this entry (starting at the bottom): INT
- *The following 2 entrees are repeated until all radial meshes are filled:*
- Number of radial zones filled by single material: INT
- Material Number: INT

Example input:

The following example describes the same core as used for example in CARD 18. (The extracts in parenthesis serves for explanation, and are not compulsory input).

- '* COMMENT'
- 'BOTTOM LAYER'
- 1 (one axial layer)
- 3 (3 radial layers)
- 1 (material number 1)
- 'TOP AXIAL LAYER'
- 1 (one axial layer)
- 2 (first two radial layers)
- 2 (Material number 2)
- 1 (one more radial layer - Last radial layer)
- 3 (Material number 3)

Notes:

The code will stop reading records when all axial and radial layers are filled. Please note that azimuthal dependence is not catered for in this input specification, but still to be added in the form of material specification method = 3.

Material definition

- COMMENT: STRING [255]
- *Repeat the following record for each material type (Matnum number of times)*
- Material Name: String[255]
- Removal cross-sections (1..G): real(8)
- Diffusion cross-sections (1..G): real(8)
- Nufission cross-sections (1..G): real(8)
- Power cross-sections (1..G): real(8)
- Scatter Matrix (1..G,1..G): real(8)

Example input:

- '* COMMENT'
- 'Top.Bot Ref 1'
- 2.80E-02 3.30E-03
- 1.0684D0 0.32051D0
- 0.0D0 0.0D0
- 1.0D0 1.0D0
- 0.0D0 2.60E-02
- 0.0D0 0.0D0
- 'FUEL type 1'
- 1.04750E-02 1.30630E-02
- 1.3052D0 0.88857D0
- 1.17760E-03 1.32680E-02
- 1.0D0 1.0D0
- 0.0D0 8.03510E-03
- 0.0D0 0.0D0

Notes:

Please note that the absorption cross-section specified should be removal cross-section, which includes out of group scattering, therefore: $\sigma_r^{g'} = \sigma_a^{g'} + \sum_{g=1,G, g \neq g'} \sigma_s^{g'}$ or equivalently

$$\sigma_{s,t,u}^g = \sigma_{s,t,u}^{g,total} - \sigma_{s,t,u}^{g \rightarrow g,scat}$$

Fixed Source specification (only given if FIXED SOURCE FLAG in CARD 13=1)

- COMMENT: STRING [255]
- Number of source zones: INT

- COMMENT: STRING [255]
- The following one line record is repeated "Number of Source zone" times
- START GROUP: INT ; END GROUP:INT; START RADIAL:INT; END RADIAL:INT
; START AXIAL: INT; END AXIAL: INT ; START AZIMUTHAL: INT ; END AZ-
IMUTHAL: INT ; SOURCE STRENGTH: real (8)

Example input:

- '* COMMENT'
- 1
- '* COMMENT'
- 1 1 1 3 4 4 1 4 1.5

Notes:

The above input describes a source of density 1.5 in group 1, placed in radial zones 1 to 3, on axial layer 4, for first 4 azimuthal zones.

Results requirement specification

- COMMENT: STRING [255]
- Number of result sets requested: INT
- COMMENT: STRING [255]
- The following one line record is repeated "Number of Result set" times
- Primary results category: STRING [255]
- Secondary results category: STRING [255]
- START GROUP: INT ; END GROUP:INT; START RADIAL:INT; END RADIAL:INT
; START AXIAL: INT; END AXIAL: INT ; START AZIMUTHAL: INT ; END AZ-
IMUTHAL: INT

Example input:

- '* COMMENT'

- 1
- '* COMMENT'
- 'FLUX'
- 'LIST'
- 1 1 1 4 6 6 1 4

Notes:

The above input requests a list of fluxes in group 1, placed in radial zones 1 to 4, on axial layer 6, for first 4 azimuthal zones. Available results requests include:

Primary: 'FLUX'

Secondary:

- 'LIST'
- 'AVERAGE'- volume-averaged flux for region
- 'RAVERAGE'-axially and azimuthally-averaged (volume) fluxes for radial regions
- 'AAVERAGE'-radially and azimuthally-averaged(volume) fluxes for axial regions
- 'AZIAVERAGE' - radially and axially-averaged(volume) fluxes for azimuthal regions
- 'RZAVERAGE' - Map of radially x axial fluxes averaged azimuthally
- 'RTHAVERAGE' - Map of radially x azimuthally fluxes averaged axially

Primary: 'POWER'

Secondary:

- 'LIST'
- 'AVERAGE'- volume-averaged power for region
- 'RAVERAGE'-axially-averaged powers listed for radial and azimuthal region
- 'AAVERAGE'-radially-averaged powers listed for axial and azimuthal region

Primary: 'XS' - cross-sections

Secondary:

- 'D'
- 'REMOVAL'
- 'SCATTER'
- 'FISSION'

Primary: 'COEFF' - finite-difference coefficients

Secondary:

- 'RADIAL'
- 'AXIAL'
- 'ARC'
- 'CENTRAL'
- 'VOLUMES'

Appendix B

DODDS BENCHMARK PROBLEM

The (r, z) published ([7] and [8]) 2-group DODDS' benchmark problem is fully described in this appendix. We first present the general material layout of this two-group eigenvalue problem.

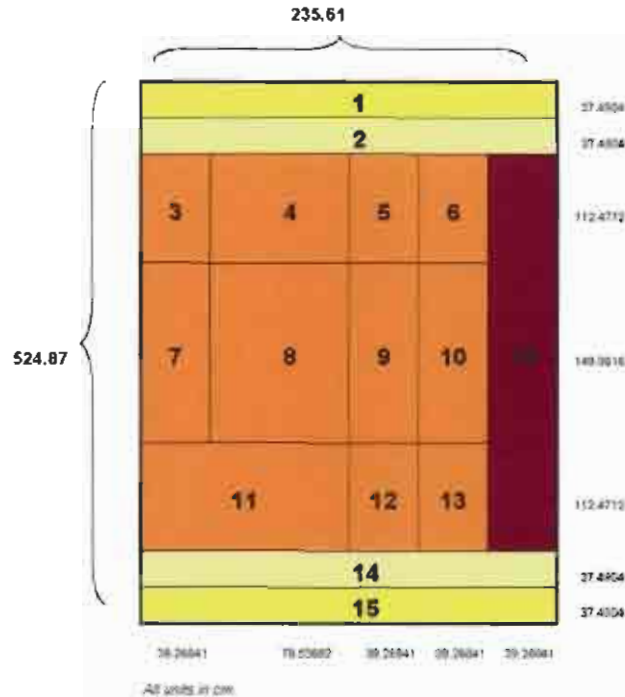


Figure B.1: DODDS' benchmark model in (r, z) geometry

Zero-flux boundary conditions are used on all outer bounding surfaces, as described in [8]. Cross-sections associated with each zone are listed in the table below.

Region	G	$D(cm)$	σ^{rem}	$v\sigma^{flr}$	$\sigma_{1,2}^{tot}$
1,15	1	1.0684	0.028	0	0.026
	2	0.32051	0.0033	0	
2,14	1	1.3495	0.01201	0	0.012
	2	0.87032	0.019	0	
3,4,11	1	1.3052	1.0475E-2	1.1776E-3	8.0351E-3
	2	0.88857	1.3063E-2	1.3268E-2	
5,12	1	1.3052	1.0475E-2	1.1776E-3	8.0351E-3
	2	0.88857	1.2623E-2	1.3268E-2	
6,13	1	1.3052	1.0475E-2	1.1776E-3	8.0351E-3
	2	0.88857	1.2183E-2	1.3268E-2	
7,8	1	1.3052	1.0475E-2	1.1776E-3	8.0351E-3
	2	0.88857	1.3435E-2	1.3268E-2	
9	1	1.3052	1.0475E-2	1.1776E-3	8.0351E-3
	2	0.88857	1.2973E-2	1.3268E-2	
10	1	1.3052	1.0475E-2	1.1776E-3	8.0351E-3
	2	0.88857	1.2933E-2	1.3268E-2	
16	1	1.2997	1.0470E-2	1.2875E-3	7.9061E-3
	2	0.87951	1.3065E-2	1.4246E-2	

Table B.1: DODDS' benchmark cross-section description

The full input of this problem to the SciFi code is given as illustration in the next appendix (Appendix C).

Appendix C

TEST CODE INPUT EXAMPLES

SciFi input example (Dodds benchmark problem)

```
** VERSION'  
  'SciFi V1.00'  
  ** TITLE'  
  'DODDS for corrected geometry RZ COMPARISON'  
  ** DATE'  
  '29/04/2004'  
  ** DESCRIPTION'  
  'Compare Cylindrical solution with ANL BENCHMARK'  
  ** PRINTOUT FILE'  
  'DODDS_bench.PRT'  
  ** MAX OUTER ITER, MAX INNER ITER, OUTER EPSILON, Extra POWER NORMALIZATION  
  FACTOR, DEBUG PRINTOUT?'  
  200 50 0.000001D0 1 0  
  ** NUMBER OF GROUPS, FIRST THERMAL GROUP'  
  2 2  
  ** Chi - fission spectrum distribution per energy group'  
  1.0D0 0.0D0  
  ** Number of Radial, Axial and Azimuthal meshes'  
  18 28 1  
  ** Albedo boundary values on outer radial boundary for group (-1 for zero-flux boundary condition)'  
  -1.0D0 -1.0D0  
  ** Albedo boundary values on bottom axial boundary for groups '  
  -1.0D0 -1.0D0  
  ** Albedo boundary values on top axial boundary for groups '  
  -1.0D0 -1.0D0  
  **Uniform mesh?, Fixed source specification'  
  1 0
```

'* if 1 then Default r,z, size for meshes, if 2 then default r,z sizes followed by overlay coarse rad mesh,
else r,z, arc deltas'

13.08947D0 18.74520D0

 '* Number of Materials used, Method of material specification, 1 - combinational, 0 - explicit'

9 1

 '* Map of material specs, per axial layer, then radial zone, per azimuthal section'

 '*BOTTOM REF'

2

18

1

 '*INNER BOTTOM REF*'

2

18

2

 '*FUEL SECTION below mid '

6

9

3

3

4

3

5

3

9

 '*FUEL SECTION mid '

8

9

6

3

7

3

8

3

9

 '*FUEL SECTION above mid '

6

9

3

3

4

3

5

3

```

9
'*INNER TOP REF'
2
18
2
'*TOP REF'
2
18
1
'* multi-group cross-sections per material - ID, Removal, Diff, NuFiss, Power, Scatter Matrix'
'Top,Bot Ref 1'
2.80E-02 3.30E-03
1.0684D0 0.32051D0
0.0D0 0.0D0
0.0D0 0.0D0
0.0D0 2.60E-02
0.0D0 0.0D0
'Inner Top,Bot Ref 2'
1.2010E-02 1.90E-02
1.3495D0 0.87032D0
0.0D0 0.0D0
0.0D0 0.0D0
0.0D0 1.20E-02
0.0D0 0.0D0
'FUEL type 3'
1.04750E-02 1.30630E-02
1.3052D0 0.88857D0
1.17760E-03 1.32680E-02
1.17760E-03 1.32680E-02
0.0D0 8.03510E-03
0.0D0 0.0D0
'FUEL type 4'
1.04750E-02 1.26230E-02
1.3052D0 0.88857D0
1.17760E-03 1.32680E-02
1.17760E-03 1.32680E-02
0.0D0 8.03510E-03
0.0D0 0.0D0
'FUEL type 5'
1.04750E-02 1.21830E-02
1.3052D0 0.88857D0
1.17760E-03 1.32680E-02
1.17760E-03 1.32680E-02

```

```

0.0D0 8.03510E-03
0.0D0 0.0D0
'FUEL type 6'
1.04750E-02 1.34530E-02
1.3052D0 0.88857D0
1.17760E-03 1.32680E-02
1.17760E-03 1.32680E-02
0.0D0 8.03510E-03
0.0D0 0.0D0
'FUEL type 7'
1.04750E-02 1.29730E-02
1.3052D0 0.88857D0
1.17760E-03 1.32680E-02
1.17760E-03 1.32680E-02
0.0D0 8.03510E-03
0.0D0 0.0D0
'FUEL type 8'
1.04750E-02 1.29330E-02
1.3052D0 0.88857D0
1.17760E-03 1.32680E-02
1.17760E-03 1.32680E-02
0.0D0 8.03510E-03
0.0D0 0.0D0
'BLANKET region'
1.04700E-02 1.30650E-02
1.2997D0 0.87951D0
1.28750E-03 1.42460E-02
1.28750E-03 1.42460E-02
0.0D0 7.90610E-03
0.0D0 0.0D0

```

'*RESULTS SPECIFICALLY REQUESTED, number of result sets'

4

'* Result descriptor, secondary descriptor (or operation), Group range, radial range, axial range, azimuthal range'

'POWER'

'LIST'

1 1 1 18 14 14 1 1

'FLUX'

'LIST'

2 2 1 18 14 14 1 1

'POWER'

'RAVERAGE'VERSION'

1 2 1 18 1 28 1 1

'POWER'
'AAVERAGE'
1 2 1 18 1 28 1 1
'INPUT END'

Appendix D

IAEA BENCHMARK DESCRIPTION (CYLINDRICAL)

As basic illustration, Figures D.1, D.2 and D.3 describe the general material layout.

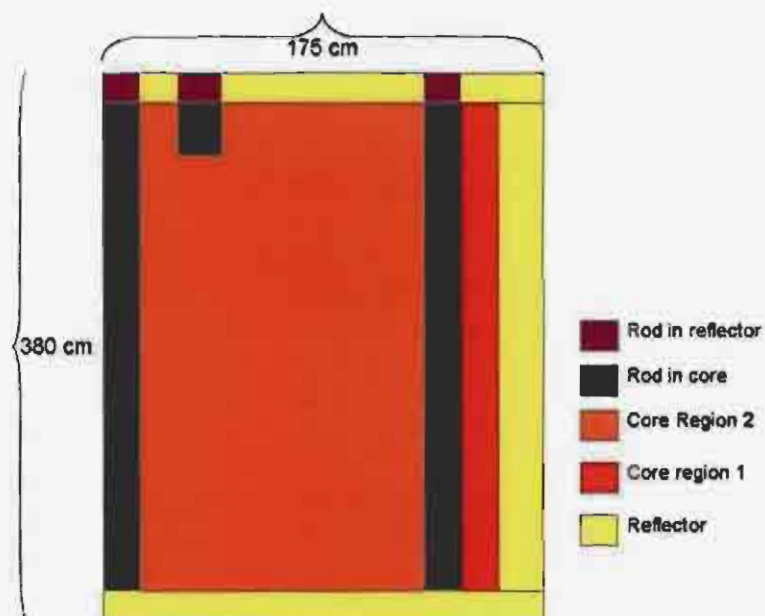


Figure D.1: IAEA (r, z) layout - azimuthal cut at 45 degrees

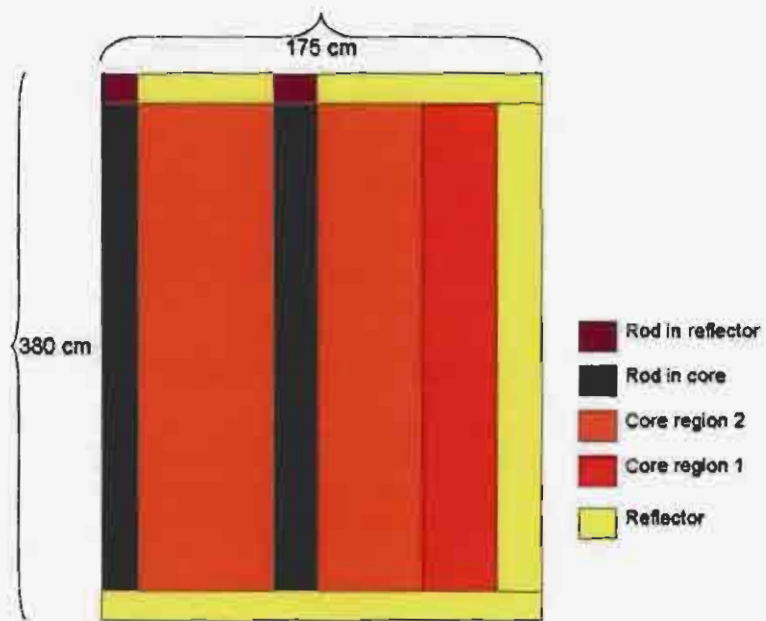


Figure D.2: IAEA (r, z) layout - azimuthal cut at 0 degrees

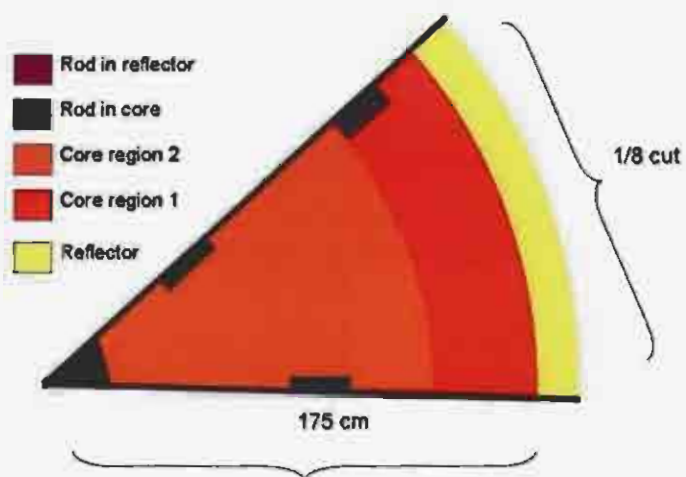


Figure D.3: IAEA (r, θ) layout - top view

The applied meshing scheme for the nodal calculation is as follows:

- Radial direction: 1.0 2.0 3.0 4.0 20 25 25 20 20 8 22 25
- Axial direction: 19 x 20
- Azimuthal direction (radians): 0.130899693 0.179987079 0.179987079 0.19634954

Graphically, the nodal mesh and material layout may be represented as in Figures D.4 and D.5 below. Four figures are presented, each representing a different axially homogeneous (r, θ) slice. For ease of representation, the (r, θ) slices are presented on an (x, y) grid, and are therefore not to scale. The four figures represent 20 cm, 260 cm, 80 cm and 20 cm axial slices (from bottom to top), respectively.

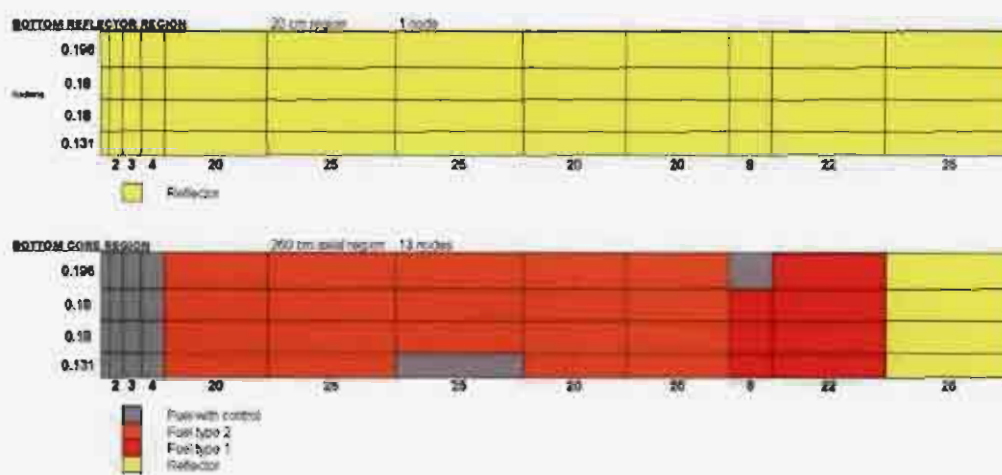


Figure D.4: IAEA Nodal mesh - bottom reflector and bottom core regions

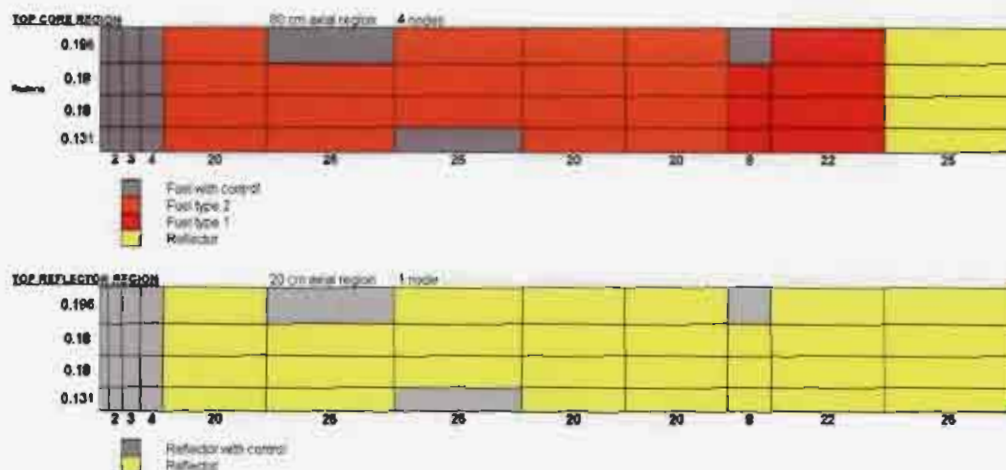


Figure D.5: IAEA Nodal mesh - top core and top reflector regions

The meshing scheme described in these figures define the mesh on which powers and fluxes are reported in Chapter 6, with the exception that the first four meshes are averaged to produce a single value for the central control rod.

Cross-sections

Five materials are utilized in this benchmark, and cross-sections are provided in this section. These cross-sections are specified in Table D.1 below:

Region	G	$D(cm)$	σ^{rem}	$\nu\sigma^{fis}$	$\sigma_{1,2}^{scat}$
Reflector	1	2.0	0.04	0.0	0.04
	2	0.3	0.01	0.0	0.0
Fuel 1	1	1.5	0.03	0.0	0.02
	2	0.4	0.08	0.135	0.0
Fuel 2	1	1.5	0.03	0.0	0.02
	2	0.4	0.085	0.135	0.0
Control/Fuel	1	1.5	0.03	0.0	0.02
	2	0.4	0.13	0.135	0.0
Control/Ref	1	2.0	0.04	0.0	0.04
	2	0.3	0.055	0.0	0.0

Table D.1: IAEA Material cross-sections

Appendix E

RECURRENCE RELATIONSHIPS FOR FLUX MOMENTS

E.1 Flux moments

We first derive recurrence relationship for integrals of exponential-polynomial form.

$$I_l = \int_{-1}^1 e^{aw} P_l(w) dw = -\frac{2l-1}{a} I_{l-1} + I_{l-2}, \quad a \neq 0 \quad (\text{E.1})$$

with

$$I_0 = \frac{2}{a} \sinh(a), \quad I_1 = \frac{2}{a} \left(\cosh(a) - \frac{\sinh(a)}{a} \right), \quad a \neq 0$$

Utilizing the relationships

$$\cosh(\beta) = \frac{1}{2} (e^\beta + e^{-\beta}) \quad \text{and} \quad \sinh(\beta) = \frac{1}{2} (e^\beta - e^{-\beta})$$

moments of one-dimensional flux are separately calculated in their *cosh*, *sinh* and particular solution components. Let us firstly define the hyperbolic cosine moments, which exist only for l even:

$$f_l^{\text{cos}} = \int_{-1}^1 \cosh(\bar{\beta}_n^{\text{nm}} w) P_l(w) dw = \frac{1}{2} \left(-\frac{2l-1}{\bar{\beta}_n^{\text{nm}}} I_{l-1}^{\text{cos},+} + I_{l-2}^{\text{cos},+} + \frac{2l-1}{\bar{\beta}_n^{\text{nm}}} I_{l-1}^{\text{cos},-} + I_{l-2}^{\text{cos},-} \right) \quad (\text{E.2})$$

$$I_0^{\text{cos},+} = \frac{2}{\bar{\beta}_n^{\text{nm}}} \sinh(\bar{\beta}_n^{\text{nm}}), \quad I_1^{\text{cos},+} = \frac{2}{\bar{\beta}_n^{\text{nm}}} \left(\cosh(\bar{\beta}_n^{\text{nm}}) - \frac{\sinh(\bar{\beta}_n^{\text{nm}})}{\bar{\beta}_n^{\text{nm}}} \right)$$

$$I_0^{\cos,-} = \frac{2}{\beta_n^{nm}} \sinh(\overline{\beta_n^{nm}}), I_1^{\cos,-} = \frac{-2}{\beta_n^{nm}} (\cosh(\overline{\beta_n^{nm}}) - \frac{\sinh(\overline{\beta_n^{nm}})}{\beta_n^{nm}})$$

$$I_l^{\cos,+} = -\frac{2l-1}{\beta_n^{nm}} I_{l-1}^{\cos,+} + I_{l-2}^{\cos,+}$$

$$I_l^{\cos,-} = \frac{2l-1}{\beta_n^{nm}} I_{l-1}^{\cos,-} + I_{l-2}^{\cos,-}$$

$$f_0^{\cos} = \frac{1}{2} (I_0^{\cos,+} + I_0^{\cos,-})$$

$$f_1^{\cos} = \frac{1}{2} (I_1^{\cos,+} + I_1^{\cos,-})$$

for

$$l = 0, 2, 4, \dots$$

Similarly define:

$$f_l^{\sin} = \int_{-1}^1 \sinh(\overline{\beta_n^{nm}} w) P_l(w) dw = \frac{1}{2} \left(-\frac{2l-1}{\beta_n^{nm}} I_{l-1}^{\sin,+} + I_{l-2}^{\sin,+} - \frac{2l-1}{\beta_n^{nm}} I_{l-1}^{\sin,-} - I_{l-2}^{\sin,-} \right) \quad (\text{E.3})$$

$$I_0^{\sin,+} = \frac{2}{\beta_n^{nm}} \sinh(\overline{\beta_n^{nm}}), I_1^{\sin,+} = \frac{2}{\beta_n^{nm}} (\cosh(\overline{\beta_n^{nm}}) - \frac{\sinh(\overline{\beta_n^{nm}})}{\beta_n^{nm}})$$

$$I_0^{\sin,-} = \frac{2}{\beta_n^{nm}} \sinh(\overline{\beta_n^{nm}}), I_1^{\sin,-} = \frac{-2}{\beta_n^{nm}} (\cosh(\overline{\beta_n^{nm}}) - \frac{\sinh(\overline{\beta_n^{nm}})}{\beta_n^{nm}})$$

$$I_l^{\sin,+} = -\frac{2l-1}{\beta_n^{nm}} I_{l-1}^{\sin,+} + I_{l-2}^{\sin,+}$$

$$I_l^{\sin,-} = \frac{2l-1}{\beta_n^{nm}} I_{l-1}^{\sin,-} + I_{l-2}^{\sin,-}$$

$$f_0^{\sin} = \frac{1}{2} (I_0^{\sin,+} - I_0^{\sin,-})$$

$$f_1^{\sin} = \frac{1}{2} (I_1^{\sin,+} - I_1^{\sin,-})$$

for

$$l = 1, 3, 5, \dots$$

E.2 Mapped flux moments

In this instance we may utilize eq. (E.1) by writing

$$e^{h_u} \cosh(\beta) = \frac{1}{2} (e^{h_u + \beta} + e^{-\beta + h_u})$$

Developing a similar recurrence relationship as in eq. (E.2), we may define:

$$(fg)_l^{\cos} = \int_{-1}^1 e^{h_u w} \cosh(\beta_n^{nm} w) P_l(w) dw = \frac{1}{2} \left(-\frac{2l-1}{h_u + \overline{\beta_n^{nm}}} I_{l-1}^{\cos,+} + I_{l-2}^{\cos,+} - \frac{2l-1}{h_u + \overline{\beta_n^{nm}}} I_{l-1}^{\cos,-} + I_{l-2}^{\cos,-} \right) \quad (\text{E.4})$$

$$I_0^{\cos,+} = \frac{2}{h_u + \overline{\beta_n^{nm}}} \sinh(h_u + \overline{\beta_n^{nm}}), \quad I_1^{\cos,+} = \frac{2}{h_u + \overline{\beta_n^{nm}}} (\cosh(h_u + \overline{\beta_n^{nm}}) - \frac{\sinh(h_u + \overline{\beta_n^{nm}})}{h_u + \overline{\beta_n^{nm}}})$$

$$I_0^{\cos,-} = \frac{2}{h_u - \overline{\beta_n^{nm}}} \sinh(h_u - \overline{\beta_n^{nm}}), \quad I_1^{\cos,-} = \frac{2}{h_u - \overline{\beta_n^{nm}}} (\cosh(h_u - \overline{\beta_n^{nm}}) - \frac{\sinh(h_u - \overline{\beta_n^{nm}})}{h_u - \overline{\beta_n^{nm}}})$$

$$I_l^{\cos,+} = -\frac{2l-1}{h_u + \overline{\beta_n^{nm}}} I_{l-1}^{\cos,+} + I_{l-2}^{\cos,+}$$

$$I_l^{\cos,-} = -\frac{2l-1}{h_u - \overline{\beta_n^{nm}}} I_{l-1}^{\cos,-} + I_{l-2}^{\cos,-}$$

$$(fg)_0^{\cos} = \frac{1}{2} (I_0^{\cos,+} + I_0^{\cos,-})$$

$$(fg)_1^{\cos} = \frac{1}{2} (I_1^{\cos,+} + I_1^{\cos,-})$$

And similarly:

$$(fg)_l^{\sin} = \int_{-1}^1 e^{h_u w} \sinh(\beta_n^{nm} w) P_l(w) dw = \frac{1}{2} \left(-\frac{2l-1}{h_u + \overline{\beta_n^{nm}}} I_{l-1}^{\sin,+} + I_{l-2}^{\sin,+} + \frac{2l-1}{h_u + \overline{\beta_n^{nm}}} I_{l-1}^{\sin,-} + I_{l-2}^{\sin,-} \right) \quad (\text{E.5})$$

$$I_0^{sin,+} = \frac{2}{h_u + \overline{\beta_n^{nm}}} \sinh(h_u + \overline{\beta_n^{nm}}), I_1^{sin,+} = \frac{2}{h_u + \overline{\beta_n^{nm}}} (\cosh(h_u + \overline{\beta_n^{nm}}) - \frac{\sinh(h_u + \overline{\beta_n^{nm}})}{h_u + \overline{\beta_n^{nm}}})$$

$$I_0^{sin,-} = \frac{2}{h_u - \overline{\beta_n^{nm}}} \sinh(h_u - \overline{\beta_n^{nm}}), I_1^{sin,-} = \frac{2}{h_u - \overline{\beta_n^{nm}}} (\cosh(h_u - \overline{\beta_n^{nm}}) - \frac{\sinh(h_u - \overline{\beta_n^{nm}})}{h_u - \overline{\beta_n^{nm}}})$$

$$I_l^{sin,+} = -\frac{2l-1}{h_u + \overline{\beta_n^{nm}}} I_{l-1}^{sin,+} + I_{l-2}^{sin,+}$$

$$I_l^{sin,-} = -\frac{2l-1}{h_u - \overline{\beta_n^{nm}}} I_{l-1}^{sin,-} + I_{l-2}^{sin,-}$$

$$(fg)_0^{sin} = \frac{1}{2} (I_0^{sin,+} - I_0^{sin,-})$$

$$(fg)_1^{sin} = \frac{1}{2} (I_1^{sin,+} - I_1^{sin,-})$$

Appendix F

EXPANSIONS FOR DOUBLE LEGENDRE INTEGRALS

In this appendix, Taylor series expansions for the moments of double Legendre integrals are developed. These quantities can not be naturally derived from recurrence relationships, and are implemented as explicit expansions as listed below. The analytic expansions are listed, and thereafter their Taylor series counterparts. In the expressions below, l and n represent the individual orders of Legendre polynomials, and c represents the mapped mesh size h_u .

$$l=0, n=0$$

$$\frac{2 \cdot \sinh(c)}{c}$$

$$l=0, n=1$$

$$\frac{2 \cdot c \cdot \cosh(c) - 2 \cdot \sinh(c)}{c^2}$$

$$l=0, n=2$$

$$\frac{2(-3 \cdot c \cdot \cosh(c) + (3 + c^2)\sinh(c))}{c^3}$$

$$l=0, n=3$$

$$\frac{2(c(15 + c^2) \cdot \cosh(c) - 3(5 + 2c^2) \cdot \sinh(c))}{c^4}$$

$$l=0, n=4$$

$$\frac{2(-5c(21+2c^2) \cdot \cosh(c) + (105+45c^2+c^4) \cdot \sinh(c))}{c^5}$$

$$l=1, n=1$$

$$\frac{2(-32 \cdot c \cdot \cosh(c) + (2+c^2) \sinh(c))}{c^3}$$

$$l=1, n=2$$

$$\frac{2(c(9+c^2) \cdot \cosh(c) - (9+4c^2) \cdot \sinh(c))}{c^4}$$

$$l=1, n=3$$

$$\frac{2(-(c(60+7c^2) \cdot \cosh(c)) + (60+27c^2+c^4) \cdot \sinh(c))}{c^5}$$

$$l=1, n=4$$

$$\frac{2(c(525+65c^2+c^4) \cdot \cosh(c) - (525+240c^2+11c^4) \cdot \sinh(c))}{c^6}$$

$$l=2, n=2$$

$$\frac{2(-6c(9+c^2) \cdot \cosh(c)) + (54+24c^2+c^4) \cdot \sinh(c))}{c^5}$$

$$l=2, n=3$$

$$\frac{2(c(450+54c^2+c^4) \cdot \cosh(c) - 3(525+240c^2+11c^4) \cdot \sinh(c))}{c^6}$$

$$l=2, n=4$$

$$\frac{2(-(c(4725+600c^2+13c^4) \cdot \cosh(c)) + (4725+2175c^2+108c^4+c^6) \cdot \sinh(c))}{c^7}$$

$$l=3, n=3$$

$$\frac{2(-6c(10+c^2)(75+2c^2) \cdot \cosh(c)) + (4500+2070c^2+102c^4+c^6) \cdot \sinh(c))}{c^7}$$

$$l=3, n=4$$

$$\frac{2(c(55125 + 7275c^2 + 180c^4 + c^6) \cdot \cosh(c)) - (55125 + 25650c^2 + 1380c^4 + 16c^6) \cdot \sinh(c)}{c^8}$$

$$l=4, n=4$$

$$\frac{2(-10c(77175 + 10500c^2 + 291c^4 + 2c^6) \cdot \cosh(c))}{c^9} +$$

$$\frac{2((771750 + 362250c^2 + 20760c^4 + 290c^6 + c^8) \cdot \sinh(c))}{c^9}$$

These expressions are prone to round-off error, and hence, if expressed in terms of Taylor series expansions, become:

$$l=0, n=0$$

$$2 + \frac{c^2}{3} + \frac{c^4}{60} + \frac{c^6}{2520} + \frac{c^8}{181440} + \frac{c^{10}}{19958400} + O[c]^{12}$$

$$l=0, n=1$$

$$\frac{2c}{3} + \frac{c^3}{15} + \frac{c^5}{420} + \frac{c^7}{22680} + \frac{c^9}{1995840} + O[c]^{11}$$

$$l=0, n=2$$

$$\frac{2c^2}{15} + \frac{c^4}{105} + \frac{c^6}{3780} + \frac{c^8}{249480} + \frac{c^{10}}{25945920} + O[c]^{12}$$

$$l=0, n=3$$

$$\frac{2c^3}{105} + \frac{c^5}{945} + \frac{c^7}{41580} + \frac{c^9}{3243240} + O[c]^{11}$$

$$l=0, n=4$$

$$\frac{2c^4}{945} + \frac{c^6}{10395} + \frac{c^8}{540540} + \frac{c^{10}}{48648600} + O[c]^{12}$$

$$l=1, n=1$$

$$\frac{2}{3} + \frac{c^2}{5} + \frac{c^4}{84} + \frac{c^6}{3240} + \frac{c^8}{221760} + \frac{c^{10}}{23587200} + O[c]^{11}$$

$$l=1, n=2$$

$$\frac{4c}{15} + \frac{4c^3}{105} + \frac{c^5}{630} + \frac{c^7}{31185} + \frac{c^9}{2594592} + O[c]^{11}$$

$$l=1, n=3$$

$$\frac{2c^2}{35} + \frac{c^4}{189} + \frac{c^6}{5940} + \frac{c^8}{360360} + \frac{c^{10}}{35380800} + O[c]^{12}$$

$$l=1, n=4$$

$$\frac{8c^3}{945} + \frac{2c^5}{3465} + \frac{2c^7}{135135} + \frac{c^9}{4864860} + O[c]^{11}$$

$$l=2, n=2$$

$$\frac{2}{5} + \frac{11c^2}{105} + \frac{c^4}{140} + \frac{17c^6}{83160} + \frac{83c^8}{25945920} + \frac{41c^{10}}{1297296000} + O[c]^{12}$$

$$l=2, n=3$$

$$\frac{6c}{35} + \frac{c^3}{45} + \frac{41c^5}{41580} + \frac{23c^7}{1081080} + \frac{c^9}{3706560} + O[c]^{11}$$

$$l=2, n=4$$

$$\frac{4c^2}{105} + \frac{34c^4}{10395} + \frac{29c^6}{270270} + \frac{c^8}{540540} + \frac{c^{10}}{50893920} + O[c]^{12}$$

$$l=3, n=3$$

$$\frac{2}{7} + \frac{23c^2}{315} + \frac{13c^4}{2772} + \frac{7c^6}{51480} + \frac{19c^8}{8648640} + \frac{c^{10}}{44553600} + O[c]^{12}$$

$$l=3, n=4$$

$$\frac{8c}{63} + \frac{8c^3}{495} + \frac{31c^5}{45945} + \frac{2c^7}{135135} + \frac{c^9}{5250960} + O[c]^{11}$$

$$l=4, n=4$$

$$\frac{2}{9} + \frac{13c^2}{231} + \frac{643c^4}{180180} + \frac{109c^6}{1081080} + \frac{79c^8}{49008960} + \frac{461c^{10}}{27935107200} + O[c]^{12}$$

Appendix G

TRANSVERSE LEAKAGE QUADRATIC FIT

We assume that the transverse leakage across three neighbouring nodes will be adequately described by a quadratic polynomial:

$$L(w) = q + rw + sw^2$$

We calculate the average leakage in each of the three nodes via

$$\frac{1}{h} \int_{-\frac{h}{2}}^{\frac{h}{2}} L(w) du$$

and let the average leakage in each of the neighbouring nodes be denoted by LA, LB and LC for nodes of sizes k, l and m respectively. We find coefficients q, r, s such that the average leakage in each of the three nodes are conserved:

$$q = \text{LB} - \frac{l^2(l(\text{LA} - 2\text{LB} + \text{LC}) + k(-\text{LB} + \text{LC}) + (\text{LA} - \text{LB})m)}{4(k+l)(l+m)(k+l+m)}$$

$$r = \frac{-2k^2(\text{LB} - \text{LC}) + l^2(-\text{LA} + \text{LC}) + 2(-\text{LA} + \text{LB})m^2 - 3l(k(\text{LB} - \text{LC}) + (\text{LA} - \text{LB})m)}{(k+l)(l+m)(k+l+m)}$$

$$s = \frac{3(l(\text{LA} - 2\text{LB} + \text{LC}) + k(-\text{LB} + \text{LC}) + (\text{LA} - \text{LB})m)}{(k+l)(l+m)(k+l+m)}$$

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