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Department of Mechanical and Nuclear Engineering

ADVANCED MULTI-DIMENSIONAL DETERMINISTIC TRANSPORT
COMPUTATIONAL CAPABILITY FOR SAFETY ANALYSIS OF PEBBLE-BED
REACTORS

A Thesis in
Nuclear Engineering

by

Bismark Mzubanzi Tyobeka

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The thesis of Bismark Mzubanzi Tyobeka was reviewed and approved* by the following:

Kostadin N. Ivanov  
Professor of Nuclear Engineering  
Thesis Advisor  
Chair of Committee

Robert M. Edwards  
Professor of Nuclear Engineering

Yousry Y. Azmy  
Professor of Nuclear Engineering

Michael Adewumi  
Professor and Quentin E. and Louise L. Wood Faculty Fellow in  
Petroleum & Natural Gas Engineering

Andreas Pautz  
Special Member  
Group Leader: Codes and Methods  
AREVA NP, Erlangen, Germany

Frederik Reitsma  
Special Member  
Group Leader: Methods and Codes Development  
Pebble Bed Modular Reactor (Proprietary, Limited)  
Centurion, South Africa

Jack Brenizer  
Professor of Nuclear and Mechanical Engineering  
Chair: Nuclear Engineering Program

*Signatures are on file in the Graduate School
A coupled neutron transport thermal-hydraulics code system with both diffusion and transport theory capabilities is presented. At the heart of the coupled code is a powerful neutronics solver, based on a neutron transport theory approach, powered by the time-dependent extension of the well known DORT code, DORT-TD. DORT-TD uses a fully implicit time integration scheme and is coupled via a general interface to the thermal-hydraulics code THERMIX-DIREKT, an HTR-specific two dimensional core thermal-hydraulics code. Feedback is accounted for by interpolating multigroup cross sections from pre-generated libraries which are structured for user specified discrete sets of thermal-hydraulic parameters e.g. fuel and moderator temperatures. The coupled code system is applied to two HTGR designs, the PBMR 400MW and the PBMR 268MW. Steady-state and several design basis transients are modeled in an effort to discern with the adequacy of using neutron diffusion theory as against the more accurate but yet computationally expensive neutron transport theory. It turns out that there are small but significant differences in the results from using either of the two theories. It is concluded that diffusion theory can be used with a higher degree of confidence in the PBMR as long as more than two energy groups are used and that the result must be checked against lower order transport solution, especially for safety analysis purposes. The end product of this thesis is a high fidelity, state-of-the-art computer code system, with multiple capabilities to analyze all PBMR safety related transients in an accurate and efficient manner.
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CHAPTER 1

INTRODUCTION

Recent research activities in the nuclear power industry and nuclear research institutes have shown that there is a renewed interest in High Temperature Reactors of pebble-bed type. Passive safety features, simplicity of operation, a stable waste form, and more efficient use of the fuel are making this reactor type a very attractive candidate for next generation nuclear power plants. Among many designs in this reactor type, the design that has thus far shown a considerable promise in terms of advancement and progress is the Pebble Bed Modular Reactor (PBMR) design. However, this reactor concept has yet to mature, particularly with regard to methods available to evaluate coupled deterministic neutronics thermal-hydraulics behavior for design and safety analysis. These methods have lagged behind the state of the art compared to other reactor technologies. This fact motivated the conception of this work: to develop more accurate and highly efficient computational tools for the design and safety evaluation of PBMRs. Such developments should incorporate coupled multi-dimensional deterministic neutron transport and thermal-hydraulics calculations that will provide enhanced analysis capabilities to be used to advance the level of maturity of this innovative reactor concept.

1.1 Background

In the pursuit of newer nuclear reactor designs, the ultimate objective for designers is the creation of fertile, state of the art computational environment in which
investigation of novel core design concepts and engineering innovations can be easily, accurately, and efficiently explored. Nuclear scientists and engineers advancing the PBMR concept, which is an exciting option for Generation IV reactors, should not be distracted by questionable validity of analysis of their innovations due to the inadequacy of current computational tools. Their time is better spent pursuing new ideas and unproven technologies, and putting these to the test using state of the art design and analysis software systems. Presently available software systems have permitted voluminous scoping calculations that established the PBMR concept as one of the most promising designs for the next generation of nuclear reactors. However, as typical in such parametric studies efficiency, e.g. turnaround time is paramount, typically at the expense of physics model accuracy and level of sophistication. Hence diffusion theory, the de facto standard in the field, has been used extensively, and indeed successfully, to delineate the conceptual validity and parameter ranges for PBMR design. This has happened despite the weakness of the diffusion theory in modeling some features of this reactor type.

1.2 Objectives

To account for transport effects that cannot be modeled accurately with diffusion theory, most notably the out-of-core control rods, and the void on top of the core in the PBMR design, a multidimensional neutronics solver based on transport theory in the coupled code environment is developed in this work. The need of equipping neutronics analysis codes with neutron transport theory capability is investigated in this work along with addressing the challenge to bring this about in an efficient and versatile manner. For
this purpose the Oak Ridge National Laboratory’s (ORNL) two-dimensional neutron transport code DORT that has a long successful history in the field is used [1]. This code system will possess both the transport and diffusion tracks to provide nuclear scientists and engineers exploring PBMR designs an enhanced, comprehensive, computational capability to address with utmost fidelity unresolved, or yet to be discovered, issues.

Secondly, one of the important safety features of a reactor system is the ability of the control system to shut the reactor down under any circumstances when needs be. The enabling quantity for this is the so-called control rod worth. In the PBMR, the control rods are situated in the side reflectors and therefore, a three dimensional analyses is necessary for accurate prediction of control rods worth. Several diffusion approximations are currently in use in order to accomplish this because of the computational costs imposed by transport methods. The latter; in spite of their massive cost in terms of computation time; are necessary especially in making the case for newer designs where little or no experimental data exists, like in the case of the PBMR. To accomplish this, the ORNL three-dimensional $S_N$ code TORT is used in this work to construct a detailed three-dimensional transport model of the PBMR to perform studies on control rod worths and to use these studies to evaluate the available diffusion approximations. These deterministic three-dimensional transport models are further benchmarked against established Monte Carlo models for accuracy checking. The ultimate objective of this activity is to develop an accurate control rod approximation, benchmarked against detailed models, which can be used with high fidelity in transient studies.

Thirdly, to evaluate both steady-state and transient transport effects in the PBMR, both the transport and diffusion tracks in DORT are coupled with THERMIX-DIREKT, a
two-dimensional HTR core thermal hydraulics code to provide the appropriate thermal hydraulics feedback. A series of transient studies, ranging from slow thermal hydraulics transients to fast reactivity transients are performed with the coupled code for purposes of verification and validation.

1.3 Organization

Chapter 2 presents a detailed account on past and current developments in the field of HTGRs. The chapter will end by discussing the specific features of the PBMR 268 MWth design, which is used as a test model in this work.

Chapter 3 discusses the unique features of HTGR physics and the calculational complexities that these features impose on conventional reactor physics methods. A further discussion on existing computational methods employed in different organizations and institutions for the design and analysis of pebble-bed reactors is also given here. This will include the relevant physics methodologies and assumptions used and the perceived deficiencies of each of the methods. The discussion will then build up to the conception of future methods and their perceived benefits, especially with regards to the unique design features of the PBMR reactor.

Chapter 4 focuses on transport-theory methods, with the idea of introducing the discrete ordinates methods code, DORT as a preferred transport method for addressing the apparent and known deficiencies of the diffusion theory-based computer codes currently used for PBMR design and analysis. A brief discussion of the underlying theory along with an introduction to time-dependent transport theory equation for transient analysis when coupled to a suitable thermal hydraulics code will be given.
In Chapter 5, the development of 2-D PBMR \( S_N \) core model and the results for the steady-state analysis of the PBMR 268MWth benchmark problem (transport versus diffusion) are presented. Chapter 6 presents the development of 3-D PBMR \( S_N \) core model and control rod worth studies conducted using this model. Chapter 7 describes the various components of the coupling scheme for DORT-TD/THERMIX, highlighting the different features added to the DORT-TD neutronics solver and to THERMIX-DIREKT in order to fully handle the PBMR 268MWth and PBMR 400MWth designs. Chapter 8 presents the verification of the new coupled-code DORT-TD/THERMIX by modeling different transient scenarios from established international benchmarks. Finally, conclusions, discussions and future work, as well as major contributions to contemporary knowledge as a result of this work are presented in Chapter 9.
CHAPTER 2

OVERVIEW OF HIGH TEMPERATURE GAS-COOLED REACTORS

2.1 Current and past developments

Worldwide, the nuclear research community has taken a keen interest in high temperature reactor technology. In Indonesia, design studies have been made of modularized, small-size HTGRs [2], and in the Republic of South Africa, there is an ongoing techno-economic evaluation and design work of a modular HTGR with a direct cycle power conversion [3]. In the Netherlands, the ministry of economic affairs had the applicability of the HTGR in the Netherlands investigated [4] and in 1997; the INCOCEN (Inherently safe COGENeration) design was presented [5], followed by the ACACIA, a 40MWth pebble-bed reactor design project. In this design, the production of both electricity and heat is foreseen, leading to an overall plant efficiency of about 90%.

In China and Japan, test reactors have been constructed and are presently operating. The HTGR-10 in China is a small HTGR (10 MWth) and is the only pebble-bed reactor in operation today [6]. The first criticality of the HTTR (30 MWth) in Japan was attained on the 10th November 1998. It uses a prismatic core to drive a steam generator. A hydrogen production facility and gas-turbine power conversion unit is under development.

In the United States, the Department of Energy (DOE) has identified the need for an upgraded energy infrastructure to meet growing demands for electric power and transportation fuels. The Generation IV project identified reactor system concepts for producing electricity that excelled at meeting the goals of superior economics, safety,
sustainability, proliferation resistance, and physical security [7]. One of these reactor system concepts, the Very High Temperature Gas Cooled Reactor System (VHTR) is also uniquely suited for producing hydrogen without the consumption of fossil fuels or the emission of the greenhouse gases. The DOE has selected this system for the Next Generation Nuclear Power Project (NGNP), a project to demonstrate emissions-free nuclear-assisted electricity and hydrogen production by 2015. The Idaho National Laboratories (INL) in Idaho Falls, USA, leads this project. The NGNP reference concept will be a helium cooled, graphite moderated, and thermal neutron spectrum reactor with a design goal outlet temperature of 950 °C or higher. The reactor core could be either a prismatic graphite block type core or a pebble bed core. The use of molten-salt is also being evaluated. The process heat for hydrogen production will be transferred to the hydrogen plant through an intermediate heat exchanger (IHX). The reactor thermal power and core configuration will be designed to assure passive decay heat removal without fuel damage during hypothetical accidents. The fuel cycle will be a once-through, very high burnup low-enriched uranium fuel cycle.

This interest in the HTGR is mainly the result of the growing demand for an enhancement of the safety characteristics of the nuclear power reactors. Furthermore, the power conversion efficiency in these reactors is higher than that of light-water reactors (LWR), leading to a more efficient use of fuel. This is the result of the higher coolant outlet temperature in the HTGR: about 900 °C compared to about 300 °C in a LWR. The HTGR can be viewed as an inherently safe reactor and this is a result of several design features:
a. The use of coated particles embedded in a graphite matrix which practically completely retain fission products up to a fuel temperature of 1600 °C, as confirmed by experiments [8]

b. The use of graphite as both moderator for neutrons and as construction material. In contrast to metals, graphite does not melt. Furthermore, its sublimation point is at a very high temperature (about 5100 K at atmospheric pressure)

c. The use of helium as coolant

d. The low power density (2 to 6 MW/ m³, compared to at least 50 MW/m³ for a LWR)

e. A continuous fuel supply in case the core consists of spherical fuel elements, limiting the excess reactivity in the core to a minimum.

One of the most important safety requirements for reactor designs is the removal of decay heat from the reactor core in the case of an accident in order to prevent serious damage to the reactor and the release of radioactivity into the environment. First of all, the HTGR core is temperature resistant, as only ceramic materials are used. Furthermore, due to the large amounts of graphite in an HTGR, the core has a very high heat storage capacity, which is retained in the case of loss-of-coolant accident. In such an accident, the combination of the large amounts of graphite and low power density ensures a self-acting decay heat removal (by thermal radiation, heat conduction and free convection) and a maximum fuel temperature that remains within an acceptable range. Hence, the HTGR excludes melting of the core and the release of radioactive fission products from the fuel and thus satisfies the requirements of catastrophe-free nuclear technology [9].
The HTGR concept is by no means new - it originated in the late 1950s. It was further developed and tested in a number of critical experiments (for example in the KAHTER facility in Germany [10]) and test reactors, like the 20 MWth DRAGON reactor in England, the 115 MWth Peach Bottom reactor in the USA, and the 46 MWth AVR pebble bed reactor in Germany [11]. The first two test reactors employed a prismatic core, whereas the core of the AVR consisted of a randomly packed bed of fuel pebbles. Later, two much larger test reactors were built: a prismatic block type HTGR in Fort St. Vrain (Colorado, USA) of 842 MWth and the THTR-300 in Uentrop-Schmehausen (Germany), a pebble-bed type HTGR of 750 MWth. These reactors demonstrated the feasibility of the HTGR concept and confirmed the favorable characteristics claimed for it.

In this work, the HTGR design under consideration is the PBMR design, the brainchild of the South African state utility ESKOM in joint partnership with Westinghouse Electric Company and the South African Industrial Development Corporation (IDC). A full description of this design is given in the next section.

2.2 The Pebble-Bed Modular Reactor

The Pebble Bed Modular Reactor (PBMR) is a high-temperature, helium-cooled, graphite moderated reactor with a multi-pass fuelling scheme. Coupled to the reactor is a power conversion unit, which comprises of a turbo-generator unit, based upon a recuperated, direct closed-circuit cycle.

In this section, the core design will be summarized specifically with the aim to provide the reader with the geometry, dimensions and all other relevant information
necessary to perform core neutronics and safety calculations. For example, this will imply that the detail design of the reactor pressure vessel (RPV), which is unimportant for the accurate modeling of the core, will not be given. The PBMR neutronics design was subjected to an extensive range of investigations over the past years to achieve an optimized layout in terms of safety, cost and proven technology. Because the design process is still continuing, this work is based on the old designs whose data is freely available to the research community. This is a reference case of the PBMR with 268 MW thermal power and the core dimension of 3.5 m in diameter and 8.5 m in height. In this design, a 2-zone fuelling version is conceptualized with about 25% of the core volume consisting of graphite spheres, loaded into the core central region. The fuel is loaded in the outlying periphery of the core. Between these two zones a mixed region is formed due to the discrete loading points. Under the given boundary conditions, the core dimensions allow a continuous thermal power rating of 268 MWth. The important characteristics of this design are outlined in Table 2-1 below:
Table 2-1: Overview of the PBMR design parameters

<table>
<thead>
<tr>
<th>Description</th>
<th>Unit</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Thermal power</strong></td>
<td>MW&lt;sub&gt;th&lt;/sub&gt;</td>
<td>268</td>
</tr>
<tr>
<td><strong>Heavy metal in fuel elements</strong></td>
<td>g/FS</td>
<td>9</td>
</tr>
<tr>
<td><strong>Target burn-up of fuel</strong></td>
<td>MWd/kg</td>
<td>80</td>
</tr>
<tr>
<td><strong>Core average height</strong></td>
<td>cm</td>
<td>852</td>
</tr>
<tr>
<td><strong>Core radius</strong></td>
<td>cm</td>
<td>175</td>
</tr>
<tr>
<td><strong>Core volume</strong> (filled with fuel and moderator elements)**</td>
<td>m&lt;sup&gt;3&lt;/sup&gt;</td>
<td>81.97</td>
</tr>
<tr>
<td><strong>Density of the pebble bed</strong></td>
<td>Pebbles / m&lt;sup&gt;3&lt;/sup&gt;</td>
<td>5 394</td>
</tr>
<tr>
<td><strong>Average number of passes through the core</strong></td>
<td></td>
<td>10</td>
</tr>
<tr>
<td><strong>Radii of modelling zones in the core:</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>• Inner zone</td>
<td>cm</td>
<td>81 (graphite only)</td>
</tr>
<tr>
<td>• Mixing zone</td>
<td></td>
<td>113</td>
</tr>
<tr>
<td>• Outer annulus</td>
<td></td>
<td>175</td>
</tr>
<tr>
<td><strong>Admixing of fuel spheres in the respective radial zones as given above</strong></td>
<td>%</td>
<td>0.5 (for modelling only)</td>
</tr>
<tr>
<td></td>
<td></td>
<td>50</td>
</tr>
<tr>
<td></td>
<td></td>
<td>100</td>
</tr>
<tr>
<td><strong>Thermal Performance:</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Primary coolant temperatures</strong></td>
<td>°C</td>
<td>536/900</td>
</tr>
<tr>
<td><strong>Mass flow rate through reactor</strong></td>
<td>kg/s</td>
<td>129</td>
</tr>
<tr>
<td><strong>Primary system pressure</strong></td>
<td>MPa</td>
<td>7</td>
</tr>
<tr>
<td><strong>RCS group 1</strong></td>
<td></td>
<td>Nine top end rods</td>
</tr>
<tr>
<td><strong>RCS group 2</strong></td>
<td></td>
<td>Nine bottom end rods</td>
</tr>
<tr>
<td><strong>Reserve Shutdown System (RSS)</strong></td>
<td></td>
<td>Seventeen Small Absorber Sphere systems</td>
</tr>
</tbody>
</table>

The PBMR uses the TRISO type fuel design. In this design, each fuel element contains coated UO<sub>2</sub> fuel particles that are uniformly distributed in a graphite matrix,
which together constitute the fuel core. The fuel core is in turn coated with a layer of graphite which serves as a cladding and moderator. The detailed UO$_2$ fuel particle (micro-sphere) specifications, and the calculated atom densities along with the fuel element overall composition, are listed in Tables 2.2 and 2.3 [12].

Table 2-2: UO$_2$ Fuel Particle Specification and Calculated Atom Densities

<table>
<thead>
<tr>
<th>Layer</th>
<th>Thickness (microns)</th>
<th>Outer Diameter (microns)</th>
<th>Density (g/cm$^3$)</th>
<th>Mass (mg)</th>
<th>$^{235}$U ($10^{23}$ cm$^{-3}$)</th>
<th>$^{238}$U ($10^{23}$ cm$^{-3}$)</th>
<th>$^{16}$O ($10^{23}$ cm$^{-3}$)</th>
<th>$^{12}$C ($10^{23}$ cm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>UO$_2$</td>
<td>-</td>
<td>500</td>
<td>10.4</td>
<td>0.703</td>
<td>2.062 $\times 10^{-3}$</td>
<td>2.192 $\times 10^{-2}$</td>
<td>4.799 $\times 10^{-2}$</td>
<td></td>
</tr>
<tr>
<td>Buffer C</td>
<td>95</td>
<td>690</td>
<td>1.05</td>
<td>0.112</td>
<td></td>
<td></td>
<td></td>
<td>5.265 $\times 10^{-2}$</td>
</tr>
<tr>
<td>IpyC</td>
<td>40</td>
<td>770</td>
<td>1.9</td>
<td>0.127</td>
<td>9.528 $\times 10^{-2}$</td>
<td>9.528 $\times 10^{-2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>SiC</td>
<td>35</td>
<td>840</td>
<td>3.2</td>
<td>0.227</td>
<td>4.782 $\times 10^{-2}$</td>
<td>4.782 $\times 10^{-2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>OPyC</td>
<td>40</td>
<td>920</td>
<td>1.9</td>
<td>0.185</td>
<td>9.528 $\times 10^{-2}$</td>
<td>9.528 $\times 10^{-2}$</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Total</td>
<td></td>
<td></td>
<td></td>
<td>1.354</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Table 2-3: Fuel element composition

<table>
<thead>
<tr>
<th></th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass Uranium per FS</td>
<td>9.0 g</td>
</tr>
<tr>
<td>Enrichment</td>
<td>8.1%</td>
</tr>
<tr>
<td>Number of Coated Particles</td>
<td>~15 000</td>
</tr>
<tr>
<td>Mass of Coated Particles</td>
<td>19.67 g</td>
</tr>
<tr>
<td>Mass of UO₂</td>
<td>10.21 g</td>
</tr>
<tr>
<td>Mass of SiC</td>
<td>3.29 g</td>
</tr>
<tr>
<td>Mass of Buffer Carbon</td>
<td>1.625 g</td>
</tr>
<tr>
<td>Mass of Pyrolytic Carbon</td>
<td>4.54 g</td>
</tr>
<tr>
<td>Density of Graphite</td>
<td>1.75 g/cm³</td>
</tr>
<tr>
<td>Mass of Graphite</td>
<td>185.4 g</td>
</tr>
<tr>
<td>Mass of Fuel Sphere</td>
<td>205.1 g</td>
</tr>
<tr>
<td>Diameter of Fuel Sphere</td>
<td>60 mm</td>
</tr>
<tr>
<td>Diameter of Fuel Zone</td>
<td>50 mm</td>
</tr>
<tr>
<td>Thickness of Graphite Fuel-Free Zone</td>
<td>5 mm</td>
</tr>
<tr>
<td>Volume of Fuel Sphere</td>
<td>113.1 cm³</td>
</tr>
</tbody>
</table>

Figure 2.1 below represents a typical PBMR core. From the figure, it is clear that fuel is loaded and flows downward through the core. The in-core flow of pebbles is based on the following assumptions:

a. Parallel flow in the upper part of the pebble bed.

b. Towards the bottom of the core the cone together with the discharge tube has an effect on the flow velocity of the pebbles. Kleine-Tebbe experimentally determined the flow patterns of pebbles during the final discharge of the THTR.
[13], which was performed without reloading of spheres. General agreement with these flow patterns was found with flow rate experiments in the AVR.

The pebble flow patterns derived by Kleine-Tebbe are deemed applicable to model the characteristics of the PBMR pebble flow in the lower core region. In the lower

Figure 2-1: PBMR 268 MWth Core
part of the core a transition from parallel flow to the flow pattern based on the THTR experiment is achievable via interpolation. In general, refueling in these reactors is achieved via loading tubes in different channels of the core as shown in Figure 2.2 below for the HTR-Modul case.

---

Figure 2-2: Fuel Batches, Core flow and shuffling scheme
For the benefit of clarity the partial volumes normally used to simulate the burnup performance of the fuel elements could be assumed equal. Twenty percent (20%) of the total core loading is inserted into the first (inner) flow channel. This should comprise of graphite spheres only. In the second flow channel 20% of the total loading is inserted as a mixture of graphite and fuel spheres (50/50). In this case a mixed region with a width of about 25 cm is assumed. The outer lying three flow channels are each being loaded with 20% of the total loading comprising fuel spheres only. After being discharged the fuel spheres are considered mixed and thereafter reloaded according to the scheme described above.

The control of the reactor is achieved by means of control rods inserted in the side reflector. There are 18 control rods in total, nine at the top end and nine at the bottom end. There is an additional 17 shutdown rods in the form of small absorber spheres, so-called SAS and these are only provided for redundancy of the design and not envisaged to be used for the shutdown of the reactor during normal operation.

2.3 Summary

This chapter presented an overview of past and present research activities in the design of HTGRs. The details and current status of each project in the respective countries was given, including the details on design and operating experience of past HTGRs. A description of the PBMR 268MWth design, highlighting details on the reactor design parameters, fuel design and other design data was also given. This design is the one on which most of the tools developed in this work will be tested. This will be done through a set of defined and established benchmark test cases.
3.1 The unique nature of HTGR physics

The calculation and analysis of an HTGR core presents challenges, which are rather different from those encountered in conventional thermal reactors. This is primarily due to its distinct design features, which demand adapted methods in computer codes in order to be able to accurately predict the behavior of such reactor cores. In the PBMR specifically, the following design features makes it quite different from other reactors:

Nominal reactor control is achieved with control rods inserted into the side reflector. The small diameter of the modular pebble-bed results in sufficient reactivity worth of these radial absorbers so that in-core absorption is not necessary. A secondary shutdown system consisting of absorber balls that falls into the reflector channels under gravity, and removed by helium blowers is also available but these are not used for power shaping or ramping. Load following is also achievable through manipulation of the helium inventory of the primary loop.

The use of graphite as moderator has both advantages and disadvantages [14]. The low absorption cross-section means a higher moderating ratio but the crystalline properties also necessitate a detailed treatment of the scattering law in physics calculations. The low parasitic absorption rate in the overall core and reflector allows the
fuel to achieve high burnup at low fuel cost but it also requires a significantly higher total heavy metal loading. A higher moderating ratio (moderator atom per fuel atom) results in more neutron absorptions by the fuel in the thermal energy range (85% vs. 70% in a PWR) [14]. However, the high temperature promotes upscattering and pushes the thermal energy peak into a range populated by a number of plutonium resonances. This effect is particularly evident at high burnups with the significant buildup of plutonium isotopes.

The use of a coated particle fuel poses the problem of the treatment of the double heterogeneity, at the macroscopic level of the pebbles, and at the microscopic level of the coated particle. This is particularly important in the calculation of the resonance absorption. Because of the homogeneous dispersion of fuel in the moderator the resonance integral in HTGRs is two to three times higher than in most other reactor types. Because of the hard neutron spectrum the treatment of some low-lying resonances (U$^{233}$, Xe$^{135}$, and Pu) becomes particularly important in this reactor type. Furthermore, because of this hard spectrum, care must be taken in the calculation of the spectrum and power distribution at the boundary between different regions (e.g. core-reflector interface). Very characteristic of this reactor type is the treatment of fuel performance limits which are not as simple as fixed melting temperatures which should not be exceeded, but depend upon a combination of fast neutron dose, temperature level and temperature gradient (this last quantity being proportional to the power density).

In general, comparing calculational methods for HTGRs and for other reactor types, one notice the greater importance of detailed spectrum calculations (it is necessary to take a large number of energy groups) but less pronounced thermal heterogeneity
effects. While diffusion theory may seem to be sufficient for the analysis of most HTGR design problems, there is a need for transport theory to be used for problems like calculations of self-shielding, control rod worths, resonance self shielding and even for the cavity at the top of the pebble-bed in the PBMR design, where diffusion theory breaks down. Another feature of the HTGRs which needs special attention and care is the fact that its moderator temperature coefficient can in some cases be positive because of the effects of the low-lying resonances and the absence of significant density coefficient (due to the transparent nature of Helium as a coolant), so that the overall coefficient, still negative, is smaller than in most water moderated reactors. The overall temperature coefficient in large HTGRs is of the order of $10^{-5}/^\circ \text{C}$ compared to $10^{-4}/^\circ \text{C}$ for water moderated reactors and $10^{-6} - 10^{-7}/^\circ \text{C}$ for fast reactors. This behavior has very serious implication to reactivity feedback effects and accurate modeling of such behavior is of paramount importance to safety.

The HTGR also differ from other conventional reactors in relation to xenon dynamics. Generally, because neutrons travel so much further in graphite than in water, the high-temperature reactors are less spatially uncoupled than other types of reactors and thus less xenon-unstable. However, their mean power density is considerably lower and their negative temperature coefficient is not quite as large as in other reactors (as pointed out above), so that more or less the same stability issues raised about other conventional reactors are encountered at similar powers. This is a purely theoretical assumption and it may not apply in the overall because reactors of the same capacity and type with different designs (fuel cycle, type of fuel loading, geometry etc) may differ greatly in relation to stability. This motivates the need to deploy advanced calculation methods to conduct in-
depth investigations concerning the stability of HTGRs against xenon oscillations. Such space and time-dependent calculations are most important in the analysis of the load following capabilities of HTGRs.

The foregoing summary gave a detailed account of the peculiarities of HTGR physics. It is clear from the above that an investment in the development of advanced computational methods to meet the demands put forth by these special characteristics is becoming a very important aspect of contemporary reactor physics. A number of computational methods have been used in the past and some are in use currently to cater for the needs of HTGRs. These methods differ from each other in many different aspects, for example the method of solution used (nodal, finite difference etc), computational domain of the problem solved (point kinetics, one dimensional, two dimensional etc), detail and accuracy of the calculation (stand-alone neutronics or thermal hydraulics versions, coupled neutronics-thermal hydraulics version) and finally, the theory and assumptions used (neutron diffusion or neutron transport theory). In the next section, these methods as applied in computer codes for use in HTGRs are described and their respective strengths and weaknesses is be discussed.

3.2 Current neutronics and thermal hydraulic analysis methods for HTGRs.

The analysis of core behavior and fuel cycle of high temperature reactors of the pebble-bed type has been carried out in different institutions using methods which differ greatly on the level of sophistication and detail of analysis. In the following sub-sections,
the evolution of these methods and their applications in current HTGR computer codes will be discussed, pointing out their respective advantages and limitations.

### 3.2.1 Thermal-hydraulic coupled to 0-D neutronics - point kinetics models

The simplest computer codes used for the analysis of nuclear reactors are those that employ the point kinetics methods. This model describes the time behaviour of the neutron population in the reactor core. When combined with the thermal hydraulic model, the point kinetics model calculates the power, which has no spatial distribution but is the integral of the reactor power. The Relap5 code is one of the well-known codes using point kinetics for the analysis of high temperature reactors. As applied in the reactor models in [15], the Relap5 code has a primary purpose to represent the thermal hydraulic cycle of a working fluid, in this case, helium in the Brayton cycle. Heat transfer from the working fluid to the enveloping structures – so-called heat structures – and the conduction towards an outer environment can be modeled using this code. With its 3-D core thermal hydraulic model, when the power distribution over the core is known, the core is divided into layers and a portion of the power is allocated to each layer according to steady-state reference conditions. During transients, the power causes a temperature variation in the layers which introduces a reactivity disturbance. Together with the xenon reactivity contribution, the resulting net reactivity is fed back into the point reactor kinetics model. The kinetics parameters of the model determine the dynamic reactor response, and the cycle starts again. As applied in [8], this method has shown to work reasonably well in the analysis of slow transients which do not have a pronounced effect
on the reactor power shape. It has also shown advantages in calculational speeds due to the simplifications of the neutronics model and due to the absence of coupling between different codes. However, as one would expect, the Relap5 point kinetics model has also proven to have some serious limitations when applied to pebble-bed reactors:

a) Heat transfer by conduction in axial direction cannot be modeled

b) Heat structure cannot have mixed boundary conditions i.e. transfer heat by conduction and convection at the same boundary as could be expected for the PBMR environment

c) Heat transfer relations for a pebble-bed geometry are not available, some approximations are made

d) Relations for the pressure drop over the pebble-bed are also not available

Although approximations are sometimes applied to address the above drawbacks, this model can only be used for scoping studies and not for detailed design and safety analysis calculations. Furthermore, this model is also subject to the major disadvantage of point kinetics in general, namely that it is not valid for transient that could result in sharp power changes, for example, control rod ejection, which is also regarded as one of the design-basis accident in the PBMR.

Another recent contribution was made by the Oak Ridge National Laboratory (ORNL) with the development of the Graphite Severe Accident Analysis Code (GRSAC) which also uses point kinetics to represent the neutron dynamics of the reactor core. GRSAC [16] is based on an approximately 30 year’s development at ORNL sponsored by DOE/NRC. It provides for detailed accident modeling for gas-cooled reactor systems. The code has a capability to perform 3-D core thermal-hydraulics for a maximum of 3000
nodes, and neutronics (point kinetics) models for anticipated transients with scram (ATWS) accidents. The 3-D thermal-hydraulic model is in hexagonal-Z geometry. The model divides the active core into ten “blocks” high plus two each for upper and lower reflectors. It can vary the nodalization of the active core – centre reflector (total of 163 radial nodes). The central reflector can either be solid graphite or pebbles. There is a built-in graphite (and metal fuel/cladding) oxidation model, and the fuel failure and fission product release options. With these features, this code is capable to model both pebble-bed and prismatic (block type) HTGR designs. Although GRSAC presents a state-of-the-art tool for accident analysis in HTGRs, it has some inherent limitations which make it less attractive for detailed design studies and safety analysis. Over and above the limitations of the point kinetics model itself, the following are other limitations of the GRSAC code:

1. Balance of plant cannot be modeled
2. Inadvertent water ingress in the core is also not modeled (although unlikely for the Brayton cycle)
3. Not capable to model the loss of Reactor Cavity Cooling System (RCCS)
4. Control rod ejection accident is not modeled.

From the discussion of the two computer codes above, it becomes clear that although point kinetics models can provide a flexible tool to performing scoping studies and preliminary safety assessment studies, they are clouded by numerous significant limitations. The limitations identified above relegate this method to the sidelines when it comes to in-depth analysis for licensing and production purposes. This therefore implies that such methods
still need to be complemented with more detailed high fidelity and accurate models such as coupled neutronics-thermal hydraulics methods as discussed in the next section.

### 3.2.2 2-D/3-D neutronics coupled to 2-D thermal-hydraulics models

In thermal reactors, the nuclear power production is coupled with spectrum-averaged cross section changes due to temperature and other feedback effects. This necessitates the need for coupled neutronics and thermal hydraulics codes so as to be able to capture such feedback effects. Amongst the reasons for this need are the following:

1. The temperature is governed by nuclear heat production, heat transport in the coolant gas, heat conductivity in the fuel and graphite, and radiation. For HTGRs, in particular the PBMR design, the large heat capacity of the graphite causes overall temperature changes to be slow. But even small temperature changes in the particles and in the inner part of the fuel elements results in sensitive feedback to the nuclear behavior or neutronics.

2. The core temperature has to be treated in a heterogeneous way. The heat produced in the coated particles is transferred very rapidly into the graphite matrix, the inner part of the spherical fuel elements. From there it is transported to the fuel elements surface, where it must be removed by the coolant gas, global heat conduction, or radiation. All these phenomena contribute strong feedback to the neutronics.
3. The cool-down transients with strongly negative moderator temperature reactivity coefficient and the occurrence of a recriticality during such cool-down and its consequences have to be analyzed.

4. The uncertainties of inherent feedback determining power production and consequently pressure increase can be strongly reduced by applying 3D neutronics models e.g. uncertainties in the spatial effects resulting from control rod insertion or ejection.

Few computer codes within the nuclear research community have capabilities to partly or wholly address the above requirements. One such program is the VSOP (Very Superior Old Programs) [17] developed many years ago in Germany with the HTGR program. VSOP is a suite of codes presently used at the Pebble-Bed Modular Reactor (Pty) Ltd (PBMR), for the design and safety analysis of the PBMR. It consists of cross-section libraries and processing routines and neutron spectrum evaluation based upon the GAM and THERMOS codes, two-dimensional (2-D) and three-dimensional (3-D) diffusion, depletion routines, in-core and out-of-pile fuel management routines, fuel cycle cost analysis, and thermal hydraulics for pebble-bed reactors. Until recently, it was the only code available for life-cycle analysis of pebble-bed reactors. The diffusion module, based on the CITATION finite difference method, calculates the full R-Z flux distribution in general using four energy groups from one-dimensional (axial) calculations. For each CITATION region the macroscopic cross sections are calculated by VSOP using the macroscopic cross sections from the applicable VSOP layers and by applying volume weighting. The VSOP layer macroscopic cross sections are determined from the microscopic cross sections obtained from GAM and THERMOS (spectrum
calculation) and the number densities (and volume fraction) of each batch of fuel in that layer. The CITATION composition mesh structure can further be refined (sub-divided) in order to obtain an accurate finite-difference diffusion solution. For HTGR studies a choice of four energy groups have proven to be sufficient, i.e. a thermal energy group with energies between 0 to 1.86 eV, two epithermal groups with energies ranging from 1.86 to 29.0 eV and 29.0 and 1.11 MeV, and a fast energy group with energies between 1.11 and 10 MeV. No provision for up-scatters have been made in the current VSOP, and therefore limiting the user to a single thermal energy group. In the void above the pebble bed calculations are performed employing adapted diffusion coefficients. Since a diffusion coefficient for each coordinate direction has been implemented the different streaming effects (depending on the relative size and shape of the void) can be adjusted.

In VSOP94, forty isotopes can be tracked explicitly in up to 200 compositions and the spectrum calculation is repeated when a significant change in the spectrum is expected. The fuel management module tracks ‘batches’ of pebble from the moment of entry into the core, through recycling, and to eventual discharge. The batches are treated as though they reside in a stationary manner in assigned sections of fuel streamlines. After each time step, they are moved discontinuously to the next region in the streamline. The module simulates shuffling (recirculation) in this manner for currently known pebble-bed designs. It has been extended to include burn up-dependent optional re-loading of pebbles and different fuel streams. The time-dependent capability allows VSOP to model changes in the fueling scheme in mid-cycle. This code is widely accepted as the most appropriate suite of codes for the design and fuel management of pebble-bed reactors. Though effective for many situations, it is two generations of codes and
methods older than the state of the art in neutronics solvers. In particular, the finite difference method like the one used in the VSOP code is significantly slower than one that uses a nodal diffusion solver and it is thus a less effective tool for frequent repetitive calculations needed for design and optimization. Another limitation of the VSOP code lies in the fact that it relies on other external auxiliary codes to fulfill some of its functions e.g. the TINTE code used to provide for kinetics calculations and this can result in uncertainties due to the data transfer between the two codes and the separate cross section libraries used.

In recognition of the limitations on codes like VSOP, a coupled code NEM-THERMIX was developed at the Pennsylvania State University. This code is a result of a combination of the nodal diffusion code NEM and THERMIX-DIREKT, a thermal hydraulics code.

NEM [18] is a 3-D multi-group nodal diffusion code developed at The Pennsylvania State University (PSU) for modeling both steady state and transient core conditions based on the nodal expansion method. This method for solving the nodal equations in three dimensions was developed by Finnemann in the early 1980s [19]. It utilizes a transverse integration procedure and is based on the partial current formulation of the nodal balance equations. The leakage term in the one-dimensional transverse integrated equations is approximated using a standard parabolic expansion using the transverse leakages in three neighboring nodes. The nodal coupling relationships are expressed in partial current formulation and the time dependence of the neutron flux is approximated by a first order, fully explicit, finite difference scheme. This method has
been shown to very efficient although it lacked the precision of the advanced nodal codes. Recently an upgrade of the method has been completed, replacing the fourth order polynomial expansion with a semi-analytical expression utilizing a more accurate approximation of the transverse leakage. The code has options for modeling of 3-D Cartesian, cylindrical and hexagonal geometry. The cylindrical option utilizes fourth-order polynomial expansions of the 1-D transverse-integrated flux distribution in the R-, Z- and θ-directions. The cylindrical option has been verified using the Dodd’s benchmark problem [20]. This code has also been tested for applicability in pebble-bed reactors through a number of steady-state core physics benchmark and was shown to be suitable for the analysis of this reactor type.

The Thermix-Direkt code [21] calculates in 2-D, the temperature distribution in the pebble-bed due to heat transport by conduction, radiation and convection (natural and forced), given a power distribution and coolant flow conditions. The code can perform both steady state and transient calculations. Relations for, for instance, the conduction or heat transfer coefficients in the pebble-bed are partly empirical, partly exact with fitted parameters. These relations have been validated by numerous experiments with the AVR test reactor in Germany. In addition, tests with non-nuclear pebble-beds in the seventies and eighties have also been utilized in order to validate the code. As the name suggest, Thermix-Direkt is a combination of two codes: Thermix, which solves the heat conduction equation for solid materials, and Direkt, which solves the equations describing heat transfer by convection. A detailed description of the method of solution used in this code will be discussed in Chapter 7.
In order to provide capability to model both steady-state and transient conditions of HTGRs of the pebble-bed type, it was necessary to devise an efficient way of coupling NEM and THERMIX-DIREKT. In the coupling process, a feedback model has been developed to account for the feedback effects of temperature and spectrum and was implemented into NEM. The four parameters of interest in the model are fuel temperature (Tf), moderator temperature (Tm), xenon feedback and spectrum (S). Two software packages have been developed as part of this new feedback model. The first package automatically generates a macroscopic cross section library for a given PBMR core model using the cross section generation code, MICROX-2 [22]. This library contains sets of microscopic 4-D cross section tables for each composition. Users can specify the ranges of the feedback parameters as well as the number of reference points themselves. Once this information is selected it is stored at the beginning of the cross section library. This information is read by NEM together with the reference cross section values. This library contains tables for transport, absorption, fission, production and scattering cross sections. The second software package reads the tables and interpolates in them to obtain the microscopic cross section values for each spectral zone (core region) and for each broad energy group. This package interacts with NEM in the following way: first, the cross section library is read once at the beginning of the calculation process and stored in the NEM arrays. During the calculation process for each spatial node of the NEM core model, four parameters representative of this node are passed to the feedback module. Using these values, four dimensional tables are then interpolated for the appropriate macroscopic cross section values. The updated macroscopic cross sections are passed back to NEM to perform core calculations, pass the power distribution to THERMIX-
DIREKT and getting the relevant thermal-hydraulics data in turn, and this calculation loop continues as shown below.

Figure 3-1: NEM-THERMIX Coupling Scheme

The coupled code system has been tested for different kinds of PBMR steady-state and transient conditions, using the PBMR-PSU-NRG PBMR 268MWth benchmark problems [23].

The list of the computer codes and analysis methods discussed above is by no means exhaustive. There are many other computer codes in use at different institutions
which are not individually discussed in this work as they fall under one of the broad categories discussed in this section.

### 3.2.3 Coupled neutron transport-thermal hydraulics codes – the future

In the previous sections, a survey of current available methods used to analyze HTGRs under both normal and accident conditions was conducted. A brief description of each method through representative computer codes was given, including their respective strengths and weaknesses. The fact established in this survey is that other than the point kinetics method, routine analyses for HTGRs nuclear power plant design are currently mainly performed using coarse-mesh nodal or fine-mesh finite difference diffusion methods, usually in up to four groups. Although these have proven to be sufficient for many design and accident scenarios and for other different types of reactors, there are clearly situations where the few-group diffusion theory approach is expected to yield results which could be improved by applying neutron transport methods. However, the computational effort to solve the transport equation for a given system is usually orders of magnitude larger than solving the same problem using the much simpler diffusion approximation. Hence it is not very surprising that even today; transport theory is almost exclusively used for steady-state investigations. This includes e.g. fuel assembly calculations, reactor design studies or shielding analyses, to name a few diverse applications of neutron transport codes. The continuing growth in computational power and the need for sound physics models that are closer to the fundamental level, especially for the novel concepts and design of Generation IV systems, for which little intuitive
experience exists, is continually pushing transport theory to the forefront of reactor applications. In the next chapter, a discussion on the justification for this move, especially for the PBMR design will be given, including an overview of neutron transport theory, as well as a survey of available methods which can be deployed for this purpose.
CHAPTER 4

REVIEW OF THE NEUTRON TRANSPORT THEORY.

4.1 Limitations of neutron diffusion theory

The one-group diffusion theory model of neutron transport plays a crucial role in reactor theory since it is simple enough to allow scientific insight, and it is sufficiently realistic to study many important design problems. The neutrons are here characterized by a single energy or speed, and the model allows preliminary design estimates. The mathematical methods used to analyze such a model are the same as those applied in more sophisticated methods such as multigroup diffusion theory, and transport theory. The neutron flux ($\psi$) and current ($J$) are related in a simple way under certain conditions. This relationship between $\psi$ and $J$ is identical in form to a law used in the study of diffusion phenomena in liquids and gases: Fick’s law[48].

In Chemistry, Fick’s law states that: “If the concentration of a solute in one region is greater than in another of a solution, the solute diffuses from the region of higher concentration to the region of lower concentration.”

The use of this law in reactor theory leads to the diffusion approximation which makes the following assumptions.

1. The cross sections in a given material region are constant(homogenized) implying a uniform medium.
2. Scattering is isotropic in the Laboratory (LAB) system
3. The neutron flux is a slowly varying function of the position.

4. Uses a one-speed, steady-state system where the neutron density is not a function of time.

Using these assumptions, it can be shown that Fick’s law for a nuclear reactor system is given by:

\[ J = -D \nabla \varphi; \] where D is the diffusion constant.

It states that the current density vector is proportional to the negative gradient of the flux and establishes the relationship between them under enunciated assumptions. It is important to note here that the gradient operator turns the neutron flux, which is a scalar quantity into the neutron current which is a vector quantity. This law states that if the gradient of the flux is negative, then the current density is positive. This means that the particles will diffuse from the region of higher fluxes to the region of lower flux through collisions in the medium. It imposes some limitations on the problem solved because of the inherent assumptions and becomes invalid, needing corrections under the following conditions:

a) **Closeness to boundaries:**

The derivation of Fick’s law assumes an infinite medium. For a finite medium, Fick’s law is valid only at points which are more than a few mean free paths from the edges of the medium. This is so, since the exponential term dies off quickly with distance, and only points of a few mean free paths from the point where the flux is computed make a significant contribution to the integral.
b) **Proximity to sources or sinks:**

It was assumed that the contribution to the flux is mostly from scattering collisions. Sources can be present. Because of the attenuation factor, however, a small number of the source neutrons will contribute to the flux if they are more than a few mean free paths from sources.

c) **Anisotropic LAB system scattering:**

Isotropic scattering in the LAB system occurs at low energies, but this is not true in general. However, Fick’s law is still valid with moderate anisotropy in scattering if a modified form of the diffusion coefficient is used, based on transport theory. Such an expression for $D$ is given by:

$$D = \frac{1}{3 \Sigma_s \left(1 - \mu\right) \left(1 - \frac{4 \Sigma_a}{5 \Sigma_s} + \ldots\right)} = \frac{1}{3 \Sigma_s \left(1 - \mu\right)} = \frac{\lambda_\mu}{3}$$

\text{4.1}

If the absorption cross section $\Sigma_a$ is much less than $\Sigma_s$, the above equation is reduced to

$$D = \frac{1}{3 \Sigma_s \left(1 - \mu\right)} = \frac{1}{3 \Sigma_s} = \frac{\lambda_\mu}{3}$$

\text{4.2}

d) **Highly absorbing media:**

In the derivation of Fick’s Law, the flux is expanded in a Taylor’s series and is assumed slowly varying. The flux however changes rapidly in strongly absorbing media. Thus Fick’s law applies to systems in which:

$$\Sigma_a \ll \Sigma_s$$
e) **Proximity to interfaces:**

The assumption of a uniform medium is used in the derivation of Fick’s law. At the boundary between two media of different scattering properties, Fick’s law is still valid, provided that the sharp change does not lead to a rapidly varying flux, which invalidates the Taylor’s series expansions of the flux, thus Fick’s law would be valid only if the second derivative of the flux does not change appreciably.

In spite of the above limitations, for most applications so far diffusion theory provided adequate performance, and when it failed to deliver the necessary accuracy, for licensing purposes for example, transport theory was deployed on a limited basis. Three features of PBMR; in particular, makes transport theory modeling a necessity:

a. The presence of the void at the top of the pebble-bed.

b. The control rods in the side reflectors invariably introduces errors in the calculations when using codes based on the diffusion theory because of the strongly absorbing material, resulting into steep flux gradients.

c. The steep gradients in the fuel-reflector interfaces

d. Neutron streaming in the control rods and SAS channels.

### 4.2 Transport theory alternatives to the diffusion theory

Having described the deficiencies of diffusion theory in the preceding section there is little doubt that the future generation of reactors will need to deploy the more
accurate but yet expensive neutron transport methods at least for reference solutions. In this section, the basics of neutron transport theory and the assumptions on which it is based are discussed. To do that, one considers the distribution of neutrons in space and angle as defined by the particle distribution function \( N(r, \Omega, t) \), such that \( N(r, \Omega, t) \, dr \, d\Omega \) is the number of neutrons in volume element \( dr \) at position \( r \) moving in the cone of directions \( d\Omega \) as depicted in Figure 4.1. An equation for \( N(r, \Omega, t) \) can be derived by considering a balance on the differential cylindrical volume element of length \( dl = v \, dt \), where \( v \) is the neutron speed, and cross section area \( dA \) surrounding the direction of neutron motion, as shown again in Figure 4.2. The rate of change of \( N(r, \Omega, t) \), within this differential volume is equal to the rate at which neutrons with direction \( \Omega \) are flowing into the volume element, less the rate at which they are flowing out of the volume element (e.g. across the right face), plus the rate at which neutrons traveling in direction \( \Omega \) are being introduced into the volume element by scattering of neutrons within the volume element from different directions \( \Omega' \) and by fission, plus the rate at which neutrons are being introduced into the volume element by an external source \( S_{ex} \), minus the rate at which neutrons within the volume element traveling in direction \( \Omega \) are being absorbed or being scattered into a different direction \( \Omega' \), resulting in the following equation:

\[
\frac{\partial N}{\partial t}(r, \Omega, t)drd\Omega = v(N(r, \Omega, t)) - N(r + \Omega dl, \Omega, t))dAd\Omega
+ \int_0^{4\pi} d\Omega' \Sigma_s(r, \Omega' \rightarrow \Omega)vN(r, \Omega', t)drd\Omega + \frac{1}{4\pi} \int_0^{4\pi} d\Omega' v\Sigma_{f}(r)vN(r, \Omega', t)drd\Omega
+ S_{ex}(r, \Omega)drd\Omega - (\Sigma_a(r) + \Sigma_s(r))vN(r, \Omega, t)drd\Omega
\]
Performing a Taylor expansion on Equation 4.3 one obtains
To evaluate the streaming term, defining the directional flux distribution

$$\varphi(r, \Omega, t) \equiv vN(r, \Omega, t)$$  \hspace{1cm} 4.5$$

And taking note of the fact that the scattering from $\Omega'$ to $\Omega$ depends only on $\Omega \cdot \Omega = \mu_0$ so that

$$\Sigma_s(r, \Omega' \rightarrow \Omega) = \frac{1}{2\pi} \Sigma_s(r, \Omega \cdot \Omega') \equiv \frac{1}{2\pi} \Sigma_s(r, \mu_0)$$  \hspace{1cm} 4.6$$

Writing $\Sigma_t = \Sigma_d + \Sigma_s$ leads to the neutron transport equation

$$- \frac{1}{v} \frac{\partial \psi}{\partial t}(r, \Omega, t) + \Omega \cdot \nabla \psi(r, \Omega, t) + \Sigma_s(r, \mu_0)\psi(r, \Omega, t) = \int_{-1}^{1} d\mu_0 \Sigma_s(r, \mu_0)\psi(r, \Omega', t)$$

$$+ \frac{1}{4\pi} \int_{0}^{4\pi} d\Omega' \psi(r_{\Omega'}, \Omega) + S_{in}(r, \Omega) \equiv S(r, \Omega)$$  \hspace{1cm} 4.7$$

The boundary conditions for Equation 4.7 are generally specified by the physical situation. For a left boundary at $r_L$ with inward normal vector $n$, such that $n \cdot \Omega > 0$ indicates inward, one of the following boundary conditions is usually appropriate:

Vacuum \hspace{1cm} $\psi(r_L, \Omega) = 0 \hspace{0.5cm} n \cdot \Omega > 0$

Incident flux known \hspace{1cm} $\psi(r_L, \Omega) = \psi_{in}(r_L, \Omega) \hspace{0.5cm} n \cdot \Omega > 0$
Reflective \( \psi(r, \Omega) = \int_0^{4\pi} \alpha(\Omega' \rightarrow \Omega) \psi(r, \Omega') d\Omega' \) where \( \alpha \) is a reflection or albedo function. It is possible to represent the neutron transport equation in various coordinate systems. Figure 4.3 shows the representation in Cartesian geometry.

Figure 4-3: Cartesian space-angle coordinate system

4.3 The time-dependent transport equation

The time-dependent neutron transport equation and the accompanying six group precursor equation can be written as follows: (the symbols and abbreviations are well-known and standard in the literature):
These equations constitute a system of partial differential equations, which describes the time-dependent behaviour of any nuclear system. However, the vast majority of transport codes can only handle the simpler steady-state equation:

\[
\frac{\partial}{\partial t} C_f(\bar{r}, t) = -\lambda_f C_f(\bar{r}, t) + \beta \int_0^\infty dE' \nu \Sigma_f(\bar{r}, E') \phi(\bar{r}, E', t) \quad l = 1,...,6
\]

4.9

Here the time-derivative and all time-dependencies have been omitted and a separate treatment of the neutron precursors is no longer necessary. The effective multiplication factor \(k_{\text{eff}}\) may be dropped, if an external, fixed source is present and the system itself is sub critical (otherwise no solution can exist). In what follows it is shown, that the solution of the time-dependent equation 4.8 can be reduced to a series of solutions of the simpler steady-state type equation 4.10.

The implicit discretisation scheme is imposed and the time derivative in equation 4.8 is approximated as follows, where \(H\) denotes the full transport operator:
\[
\frac{1}{v} \frac{\partial}{\partial t} \psi(\bar{r}, \bar{\Omega}, E, t) = \psi(t + \Delta t) - \psi(t) = \frac{\psi^{(n+1)}(n+1) - \psi^{(n)}}{v \Delta t} = H^{(n+1)} \psi^{(n+1)}
\]

4.11

A similar relation holds for the six precursor equations. Inserting this expression in equations 4.9 and 4.10 and sorting by indices \( n \) and \( n+1 \) yield:

\[
-\bar{\Omega} \cdot \nabla \psi^{(n+1)}(\bar{r}, \bar{\Omega}, E) + \left( \sum_{\psi} + \frac{1}{v \Delta t} \right) \psi^{(n+1)}(\bar{r}, \bar{\Omega}, E) = \int dE' \int d\bar{\Omega}' \sum_{\psi} (\bar{r}, E' \rightarrow E, \bar{\Omega}' \rightarrow \bar{\Omega}) \psi^{(n+1)}(\bar{r}, \bar{\Omega}', E') +
\]

\[
\left[ \chi_p(E)(1 - \beta) + \sum_{i=1}^{6} \chi_i' (r, E) \right] \int dE' \nu \Sigma_f (\bar{r}, E') (1) + \left( \sum_{i=1}^{6} \chi_i' (r, E) \right) C_i^{(n)}(n) + \frac{1}{v \Delta t} \psi^{(n)}(\bar{r}, \bar{\Omega}, E)
\]

4.12

This is nothing else but the steady-state transport equation for the fluxes \( \psi^{(n+1)} \) with a modified total cross section, a modified fission spectrum and a “time source” term, which comprises of the fluxes and precursors of timestep \( n \). These quantities have already been calculated in the previous time step and are thus known at timestep \( n+1 \).

After solving Equation 4.12 for \( \psi^{(n+1)} \) and \( \phi^{(n+1)} = \int d\Omega \Psi^{(n+1)} \) the precursors for time step \( n+1 \) are obtained from the following relationship

\[
C_i^{(n+1)} = \frac{1}{\Delta t} \gamma_i C_i^{(n)} + \beta_i \gamma_i \int dE' \nu \Sigma_f (r, E') \Phi^{(n+1)}
\]

Defining a modified total cross section, a modified fission spectrum and a new source distribution one gets:

\[
\Sigma_i' = \Sigma_i + \frac{1}{v \Delta t}
\]

\[
\chi'(r, E) = \chi_p(r, E) (1 - \beta) + \sum_{i=1}^{6} \chi_i'(r, E) \gamma_i \beta_i \quad \text{and}
\]

\[
q_{\text{extern}}(r, \Omega, E) = q_{\text{extern}}(r, \Omega, E) + \sum_{i=1}^{6} \chi_i'(r, E) \gamma_i \beta_i \frac{1}{\Delta t} C_i^{(n)}(r) + \frac{1}{v \Delta t} \Psi^{(n)}(r, \Omega, E)
\]
Therefore, the extension of a steady-state transport to time-dependence is a simple exercise. In principle, the only changes to be made are to develop a fixed-source term for each timestep, to modify the total cross section and fission spectrum appropriately and call the transport code for each time step over and over again. Additionally, feedback effects can be accounted for by allowing the cross sections to be explicit functions of time, i.e. by varying them at each time step as well. The main drawback of this implicit scheme is the fact that each timestep will be as expensive to solve as the steady-state problem. If already the steady-state equation of the system under consideration is difficult to solve, a transient with possibly thousands of time steps will normally take an unacceptable amount of computing time.

There are several computational methods available to treat the neutron transport equation. Among others, there is the spherical harmonics method or \( P_L \), in which approximation is developed by expansion of the angular flux and the differential scattering cross section cross section in Legendre polynomials. There is also the discrete ordinates method which is based on the evaluation of the transport equation at a few discrete angular directions, or ordinates and the use of quadrature relationships to replace scattering and fission neutron source integrals over angle with summation over ordinates. Thirdly, there is the Monte Carlo method, which directly simulates neutron transport as a stochastic process. Other methods include the Method of Characteristics and of course the diffusion approximation of the transport equation.

A number of neutron transport codes have always been used in nuclear engineering for mostly time-independent or systems in steady-state, for example,
shielding calculations or just steady-state core calculations. With the advancing sophistication in computational nuclear methods it is desirable to implement the more accurate, multigroup transport approach as part of a coupled code system, on a long-term basis. Throughout the literature, the number of available time-dependent transport codes is very limited. Four recent examples are TDKENO [24] and TDTORT [25], which both use the improved quasistatic method, as well as EVENT [26] and PARTISN [27] which uses implicit or semi-implicit time integration schemes. Only codes using the quasistatic approach have also been considered in the framework of coupled reactor safety analyses, one example being the SIMMER-III-DANTSYS [28, 29] system. To add to this list, this work, seeks to rectify the deficiencies of current code systems by installing a transport theory neutronics solver as an option in the NEM-THERMIX coupled code employing a fully implicit, time discretisation scheme and the classical Discrete Ordinates method, as it is implemented in the well-known computer code DORT (Oak Ridge National Laboratories). The decision to use a deterministic code instead of a Monte-Carlo program was motivated by the fact that only the deterministic approach can provide the numerical accuracy required in time-dependent calculations. Stochastic methods, in contrast, always suffer from inherent uncertainties, which would make the analysis of e.g. slow reactivity transients unfeasible. It should further be emphasised, that the use of a fully implicit scheme in conjunction with transport theory in pebble-bed reactors is up to now rather unique and is essentially free from any additional approximations, as opposed to the popular quasistatic approaches.
4.4 Discrete Ordinates Methods

In the preceding section, a formal background of extending a steady-state transport equation to treat time-dependent problems as well as a brief overview of available computational methods to treat the transport equation was described. It was also noted that for time-dependent transport applications, the classical Discrete Ordinates (SN-) approach compares superior to other methods, which e.g. implement integral transport methods or the P_N-formulation of the transport equation. The discrete ordinates methods are based on a conceptually straightforward evaluation of the transport equation at a few discrete angular directions, or ordinates and the use of quadrature relationships to replace scattering and fission neutron source integrals over angle summations over ordinates. The essence of the methods is the choice of ordinates, quadrature weights, differencing schemes and iterative solution procedures. To illustrate the discrete ordinates formulation, one considers a simple configuration, the slab geometry. The within-group slab geometry transport equation is given by:

\[
\frac{\partial}{\partial x} \phi(x, \mu) + \sigma(x) \phi(x, \mu) = \sum_{l=0}^{L} (2l + 1) P_l(\mu) \sigma_l(x) \phi_l(x) + s(x, \mu),
\]

where \( \phi(x, \mu) \) denotes the angular flux which depends on position and \( x \) and angular variable \( \mu \), (the directional cosine of the angle considered). \( \sigma(x) \) is the total cross section and \( \phi_l(x) \) is the flux moment, and \( s(x, \mu) \) is the fission and/or external source. The Legendre moments are given by:
\( \phi_j(x) = \frac{1}{2} \int_{-1}^{1} d\mu P_j(\mu) \varphi(x, \mu) \) and the expansion of the scattering kernel have been truncated after \((L+1)\) terms, assuming adequate approximation of the kernel with that number of terms.

The discrete ordinates approximation consists of requiring equation 4.8 above to hold only for a number of distinct angles \((\mu_n)\) and then applying a compatible quadrature approximation to the integral term so that:

\[
\mu \frac{d}{dx} \varphi_n(x) + \sigma(x) \varphi_n(x) = \sum_{l=0}^{L} (2l+1) P_l(\mu_n) \sigma_l(x) \phi_l(x) + s(x, \mu_n), \tag{4.14}
\]

The angles are chosen so that the ordinates may be used to evaluate the flux moments \(\phi_j(x)\) by a quadrature formula. Thus if a quadrature formula on the interval \(-1 \leq \mu \leq 1\) with \(N\) ordinates \(\mu_n\) and corresponding weights \(w_n\) is chosen, a discrete ordinates approximation of order \(N\) is said to be the result [30]. In discrete ordinates equations, the scalar flux is approximated by a quadrature formula:

\[
\phi(x) = \frac{1}{2} \sum_{n=1}^{N} w_n \varphi_n(x) \tag{4.15}
\]

and similarly the Legendre moments by

\[
\phi_l(x) = \frac{1}{2} \sum_{n=1}^{N} w_n P_l(\mu_n) \varphi_n(x) \tag{4.16}
\]

where \(w_n > 0\), and the quadrature formula is normalized by \(\sum_n w_n = 2\).

It is convenient to choose ordinates and quadrature weights that are symmetric about \(\mu = 0\), since ordinarily right and left particle flow are of equal importance. This can be accomplished by choosing
\[ \mu_{N+1-n} = -\mu_n \quad \mu_n > 0, \quad n = 1, 2, \ldots, N/2, \quad w_n > 0, \quad n = 1, 2, \ldots, N/2 \]

With such even ordinates, reflective boundary conditions are simply prescribed:

\[ \psi_n = \psi_{N+1-n} \quad n = 1, 2, \ldots, N/2 \]

Incident flux and vacuum boundary conditions (when \( \psi_{in}(\mu) = 0 \) are given as:

\[ \psi_n = \psi_{in}(\mu_n), \quad n = 1, 2, \ldots, N/2 \]

Normally, an even number of ordinates is used (N= even), because this results in the correct number of boundary conditions and avoids certain other problems encountered with N = odd. In spite of these restrictions, there remains considerable freedom in the choice of ordinates and weights.

When cross sections are defined to be constant over \( x_{i-1/2} < x < x_{i+1/2} \), Equation 4.13 for each ordinate, can be integrated over \( x_{i-1/2} < x < x_{i+1/2} \) to obtain:

\[
\mu_n \left( \psi_n^{i+1/2} - \psi_n^{i-1/2} \right) + \sum^i \psi_n^i \Delta_i = \Delta_i Q_n^i
\]

\[ \equiv \Delta_i \left[ \sum_{l=0}^{L} \frac{2I_l + 1}{2} \Sigma_{sf} \phi^l + S^i(\mu_n) \right] \quad 4.17 \]

Where \( \psi_n^i \equiv \psi(x_i, \mu_n) \) and \( \Delta_i = x_{i+1/2} - x_{i-1/2} \). Using the diamond differencing relation \( \psi_n^i = \frac{1}{2} \left( \psi_n^{i+1/2} + \psi_n^{i-1/2} \right) \) one can specify the algorithm for sweeping to the right in the direction of neutrons travelling with \( \mu > 0 \) as:
\[
\psi_n^i = \left(1 + \frac{\Sigma_i}{2|\mu_n|}\right)^{-1}\left[\psi_n^{i-1/2} + \frac{\Delta_i Q_n^i}{2|\mu_n|}\right],
\]

\[
\psi_n^{i+1/2} = 2\psi_n^i - \psi_n^{i-1/2}
\]

As already mentioned, one of the well-known computer codes that employ the discrete ordinates methods is DORT. This is a two-dimensional code (it also has a 1-D slab option) that is suitable for \(x-y\), \(r-z\), or \(r-\theta\) geometry. It can be used to solve either the forward or the adjoint form of the Boltzmann transport equation. The Boltzmann transport equation is solved, using either the method of discrete ordinates or diffusion theory approximation. In the discrete ordinates method, the primary mode of operation, balance equations are solved for the flow of particles moving in a set of discrete directions in each cell of a space mesh and in each group of a multigroup energy structure. Iterations are performed until all implicitness in the coupling of cells, directions, groups, and source regeneration has been resolved. Several methods are available to accelerate convergence i.e., single group-wise rebalance factor, diffusion acceleration, and partial current rebalance. Anisotropic cross sections can be expressed in a Legendre expansion of arbitrary order. Output data sets can be used to provide an accurate restart of a previous problem or to deliver information to other codes. Several techniques are available to remove the effects of negative fluxes caused by the finite difference approximation and of negative scattering sources due to truncation of the cross-section expansion. The space mesh can be described such that the number of first-dimensional \((i)\) intervals varies with the second dimension \((j)\). The number of discrete directions can vary across the space mesh and with energy. Direction sets can be
biased, with discrete directions concentrated such as to give fine detail to streaming phenomena. The time-dependent version of DORT which is used in this work was developed by Pautz and Birkhofer [31] and lead to the conception of the DORT-TD code and will be discussed in Chapter 7.
5.1 Parametric Studies

In order to make a case for the need of using advanced deterministic transport methods for both steady-state and transient analysis of high temperature reactors of pebble-bed type, using the PBMR as a case in point, a transport model of the PBMR core was developed using the DORT code. When nuclear data has been reliably computed, the accuracy of an $S_N$ calculation is impacted by spatial discretization, angular quadrature and energy group structure. To optimize the developed model in terms of accuracy and efficiency, parametric studies were carried out on these three parameters. The PBMR 268MW Benchmark Problem [32] provides the test cases for this study. The reference design for this benchmark problem is derived from the PBMR 268MW design. Several simplifications were made to the design in this specification in order to limit the need for any further approximations to a minimum. The simplifications make the core design essentially two-dimensional ($r,z$). It includes flattening of the pebble bed’s upper surface and the removal of the bottom cone and de-fuel channel that results in a flat bottom reflector. Flow channels within the pebble bed have been simplified to be parallel and at equal speed while the dynamic central column and mixing zone widths were defined to be constant over the total axial height. Control rods in the side reflector are modeled as a cylindrical skirt (also referred to as a grey curtain) with a given B-10 concentration.
The modeled test cases are variations of Cases N1 and N2 in the benchmark specification. Case N1 uses fresh fuel (9 grams HM and 8% enriched) at cold conditions (300K). Case N2 is the equilibrium core of the PBMR but with fewer isotopes (some fission products excluded). Participants in this benchmark were required to use their own cross-sections. For purposes of this study, cross sections were generated using the MICROX-2 code. Seven groups’ cross sections were generated for the transport calculations (DORT) and then for the diffusion calculations (NEM), only two group’s cross sections were used. Upscatter is also treated in MICROX-2 and hence used in DORT. It should be noted here that the NEM version used in these studies is the one that
does not employ a correction for the void region, i.e. it simply approximate a void region cross section by using the graphite cross section and “diluting” them by a factor of 1000.

Since Case N2 of the benchmark is an equilibrium case, it is an interesting case on which these parametric studies can be performed. For all the parametric studies carried out, P₃ scattering order was used as it is expected that it would yield more accurate results. The parametric studies performed are summarized in the next sections.

5.1.1 Studies on angular quadrature set

Quadrature order is the first parameter investigated because it has a bearing on both accuracy and computational time (efficiency) of the calculation. With P₃ scattering order and 7-energy group cross sections, eight different fully symmetric quadrature orders were used in separate calculations, namely, P₁S₂, P₁S₄, P₁S₆, P₃S₈, P₃S₁₀, P₃S₁₂, P₃S₁₄ and P₃S₁₆. From the results shown in Figure 5.2, Figure 5.3 and Table 5.1, it can be seen that the eigenvalue, axial power and flux distribution in DORT change very slightly as the result of varying angular quadrature, especially after S₄. This is important because the higher the angular quadrature order, the longer it will take for the solution to converge, and therefore resulting in long computational times. For comparison purposes, the NEM results were also included in the figures and table above and there is a visible shift between NEM and DORT fluxes and powers. The eigenvalue compares reasonably well between transport and diffusion for this case. The cause of these differences in power and flux will be investigated in the later sections.
Table 5-1: $K_{eff}$ Results of Studies on Angular Quadrature

<table>
<thead>
<tr>
<th>Order</th>
<th>$K_{eff}$</th>
<th>Difference (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$P_3S_2$</td>
<td>1.05817</td>
<td>-41</td>
</tr>
<tr>
<td>$P_3S_4$</td>
<td>1.05859</td>
<td>1.5</td>
</tr>
<tr>
<td>$P_3S_6$</td>
<td>1.05862</td>
<td>-0.8</td>
</tr>
<tr>
<td>$P_3S_8$</td>
<td>1.05861</td>
<td>0.02</td>
</tr>
<tr>
<td>$P_3S_{10}$</td>
<td>1.05861</td>
<td>0.02</td>
</tr>
<tr>
<td>$P_3S_{12}$</td>
<td>1.05860</td>
<td>0.85</td>
</tr>
<tr>
<td>$P_3S_{14}$</td>
<td>1.05863</td>
<td>-2.04</td>
</tr>
<tr>
<td>$P_3S_{16}$(reference)</td>
<td>1.05861</td>
<td>n/a</td>
</tr>
<tr>
<td><strong>NEM</strong></td>
<td>1.06017</td>
<td>-147</td>
</tr>
</tbody>
</table>
Figure 5-2: Axial Power Distribution for Case N2 (Studies on Quadrature Order)

Figure 5-3: Axial Flux Distribution for Case N2 (Studies on Quadrature Order)
5.1.2 Studies on spatial discretization/nodalization

Using a very fine mesh in calculations can be an incentive in the sense that it yields very accurate results, but this comes at a cost of computation time especially during transients. Conversely, coarser mesh can accelerate the calculations at the expense of accuracy. To obtain an optimum nodalization while preserving accuracy and saving in computational time sensitivity studies were carried out on this parameter. With the $P_1S_4$ quadrature and scattering orders, four variations from the base case, consisting in total of 29025 meshes, were chosen, namely:

- Axial discretization only (reducing the number of nodes for each region in the axial direction by half)
- Radial discretization only (reducing the number of nodes for each region in the radial direction by half)
- Both axial and radial discretization (reducing the number of nodes for each region in both the axial and radial directions by half)
- Both axial and radial discretization (doubling the number of nodes for each region in both the axial and radial directions)
### Table 5-2: $K_{\text{eff}}$ results for Case N2 (Studies on spatial discretization)

<table>
<thead>
<tr>
<th>NODALIZATION</th>
<th>$K_{\text{eff}}$</th>
<th>Diff (pcm)</th>
<th>CASE</th>
</tr>
</thead>
<tbody>
<tr>
<td>29025 meshes, (135(r), 215(z))</td>
<td>1.05859</td>
<td>n/a</td>
<td>reference</td>
</tr>
<tr>
<td>14512 meshes, 135 (r), 107 (z)</td>
<td>1.05859</td>
<td>0</td>
<td>½ axial</td>
</tr>
<tr>
<td>14512 meshes, 67.5 (r), 215 (z)</td>
<td>1.05860</td>
<td>-0.4</td>
<td>½ radial</td>
</tr>
<tr>
<td>7256 meshes, 67.5 (r) 107 (z)</td>
<td>1.05860</td>
<td>-0.4</td>
<td>½ both</td>
</tr>
<tr>
<td>58050 meshes, 270 (r), 450(z)</td>
<td>1.05862</td>
<td>-2.68</td>
<td>Double both</td>
</tr>
</tbody>
</table>

---

**Figure 5-4**: Axial Power Distribution for Case N2 (Studies on Spatial Discretization)
From the above results again it can be seen that eigenvalue, powers and fluxes in DORT are not affected much by the change in nodalization for this benchmark problem. This is good because this means that even coarser mesh can yield accurate results and thereby reducing the computational time. However, the shift in the powers and fluxes between NEM and DORT still remains, although it looks reduced for some cases.
5.1.3 Studies on energy group structure

DORT calculations were performed with three different energy group numbers namely: 4 groups, 7 groups and 13 groups with control rods fully inserted. The boundaries (cut-off points) for these group structures are as follows respectively: 1.000E+07 1.11090E+05 2.90232E+01 2.38237E+00 0.00 (eV) for the 4 group structure, 1.000E+07 1.11090E+05 7.1017400E+03 2.90232E+01 2.38237E+00 1.85539E+00 0.0 (eV) for the 7 group structure, and 1.000E+07 3.678E+06 1.11090E+05 7.1017400E+03 130.07 2.90232E+01 8.3153 2.38237E+00 1.85539E+00 0.625 0.200 0.075 0.0 (eV) for the 13 group structure. The choice of these group structures was motivated by both the physical phenomenon (physics) and experience gained from the THTR and AVR research reactors. Performing group sensitivity studies is a necessary exercise because in transient studies, a large number of energy groups for a coupled code makes the calculation almost impossible due to high computational costs. The results of the investigation are shown below:

Table 5-3: Eigenvalue results for Case N2 (Studies on energy group structure)

<table>
<thead>
<tr>
<th>CASE</th>
<th>Keff (Rods partially inserted)</th>
<th>Keff (Rods fully inserted)</th>
<th>Differential CRW (pcm/cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 - energy groups</td>
<td>1.058310 (-138.7 pcm)</td>
<td>0.922449 (+536.4 pcm)</td>
<td>19.75</td>
</tr>
<tr>
<td>7 – energy groups</td>
<td>1.058538 (-115.9 pcm)</td>
<td>0.920801 (+371.6 pcm)</td>
<td>20.02</td>
</tr>
<tr>
<td>13 – energy groups (Reference)</td>
<td>1.059697</td>
<td>0.917085</td>
<td>20.70</td>
</tr>
</tbody>
</table>
From the results in Table 5.4 and Figure 5.6 above, two things can be observed, namely, that for the eigenvalue, there is a significant change as one increases the number of energy groups. The overall difference of 5% is observed in the differential control rod worth between 4 groups and 13 groups. The trend seems to be that as one increases the energy groups, this difference may increase but this was not pursued further in this study. However, for the power distribution, the differences are quite small, except at the edges of the core, where there are slightly increased differences due to the treatment of the graphite reflector in different energy groups, i.e. for 13 energy group there is a better treatment of the scattering properties of graphite in the edges of the core (reflector regions), hence the small peak, which is due to the neutrons “pile-up” as they are scattered back into the core. It must also be noted that the “bumps” in the power distribution curves is nothing physical but a result of a very fine mesh used in DORT,
which makes the transition from one material axial region with different burnup from the previous one very pronounced.

5.1.4 Conclusions from 2-D $S_N$ Parametric Studies

From the results of the parametric studies shown above, one can summarily draw the following conclusions:

Very little change in the eigenvalue, fluxes and power for DORT as one changes the quadrature order, especially after $S_4$. Using $S_4$ as the representative quadrature for this problem is a reasonable approximation.

There are also very small effects on power shape, fluxes and eigenvalues due to spatial discretization.

There is very little effect on the powers and the 5% difference in control rod worths between 4 groups and 13 groups can be tolerated and will be investigated later when the need arises.

There is a shift in both fluxes and power between NEM and DORT for all parametric studies carried out and the next section will deal with this observation.

5.2 Evaluation of PBMR Transport Effects in 2-D

In order to investigate the two-dimensional transport effects in the PBMR, studies were performed to isolate different effects. The first study was to investigate the effects of void cavity at the top of the pebble-bed by modeling cases with and without this feature. The
second study was to investigate the effect of control rods by modeling cases with control rods partially inserted and fully inserted. For cases where the void region was excluded, the material composition of this region was replaced with a layer of graphite. All these studies were performed with $P_1S_4$ angular quadrature, 7-energy groups and 29025 meshes ($135(r), 215(z)$). Calculations were performed 900K temperature conditions, and the results are provided below.

Table 5-4: Void transport effects with control rods fully inserted

<table>
<thead>
<tr>
<th></th>
<th>With the void region modeled</th>
<th>Void replaced by graphite</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Keff value</td>
<td>Keff value</td>
</tr>
<tr>
<td></td>
<td>NEM</td>
<td>DORT</td>
</tr>
<tr>
<td>900K</td>
<td>0.924114</td>
<td>0.920762</td>
</tr>
</tbody>
</table>

Table 5-5: Control and void effects sensitivity studies

<table>
<thead>
<tr>
<th>CASE</th>
<th>DORT (Keff)</th>
<th>NEM (Keff)</th>
<th>Difference (pcm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>No rods (with void)</td>
<td>1.07808</td>
<td>1.07996</td>
<td>-175 pcm</td>
</tr>
<tr>
<td>No rods no void</td>
<td>1.080143</td>
<td>1.08171</td>
<td>-145 pcm</td>
</tr>
</tbody>
</table>
From Figure 5.7 above, it is observed that removing the rods does not address the shift in the power distribution between transport and diffusion theory results. Note that the NEM calculations were performed with a rather coarser mesh, since it is expected that nodal methods should still yield accurate results even with coarse mesh. Subsequently this mesh was refined, to make sure that the shift does not come from mesh effects. In this way, the central graphite column (originally 78.63 cm) was divided into four nodes of 19.65 cm radially; the same was done for the mixing zone, the fuel regions and the graphite side reflector. The calculations were done with control rods fully inserted and fully withdrawn, to also investigate if the shift has anything to do with control rods. For
both these instances, the void was modeled, i.e. as a layer of helium and not replaced with a graphite layer. The results are shown below:

Figure 5-8: Axial Power Distribution (Studies on control and void effects with finer mesh)

Figure 5-9: Axial Power Distribution for Case N2 (Studies on control and void effects with finer mesh)
As confirmed by the results below, it appears that mesh effects played a significant role in the power shift between DORT and NEM. However, even with finer mesh in nodal diffusion, the presence of the void causes a shifting in the power. At this point, control rods can also be eliminated as the cause of this shift because as seen in Figure 5.8 and Figure 5.9, the shift still remains regardless of the presence or absence of control rods. When control rod and the void are completely eliminated from the model, there is an excellent agreement between diffusion and transport theory results as shown in Figure 5.10 below:

![Axial Power Distribution CaseN2@900K Void, Control Rods and Mesh Sensitivity Studies](image)

Figure 5-10: Axial Power Distribution for Case N2 (Studies on control and void effects with finer mesh)

In Figure 5.10 where a fine mesh nodal diffusion method (NEM) is compared with transport (DORT), the power at the top of the core around the void region, is observed to have been over-predicted by diffusion theory. In the void region, the only material present is helium gas, which is a “transparent” gas, and hence no interactions are
expected. Neutron streaming causes the leakage out of the system at this region to be higher. One would therefore expect the flux to be just about flat or decreasing, hence the power curve is expected to be as predicted by DORT at the void region. Diffusion theory on the other hand over-predicts the flux (and hence the power) suggesting that some phenomena is taking place in this region, which is obviously a misrepresentation. This effect is expected to be more pronounced during transients, as peak power occurrence can be wrongly predicted in diffusion theory. This justifies the development of a coupled neutronics-thermal hydraulics transport theory-based code system, which can be used to provide reference solutions for benchmarks and to investigate the transport effects present in the PBMR design. As mentioned in the introduction, another transport effect in the PBMR core is the presence of control rods in the side reflector, where three-dimensional modeling is necessary. In the preceding investigations, the control rods were approximated as a cylindrical grey curtain with a given Boron-10 concentration. In the next section, an effort has also been made on developing transport models to investigate the issues of accurate modeling of control rods.
CHAPTER 6
EVALUATION OF 3-D PBMR TRANSPORT EFFECTS

The failure of diffusion theory to model highly absorbing regions is well known and numerous methods have been developed to overcome it by using the so-called equivalent diffusion parameters. In the PBMR design, the positioning of these highly absorbing regions in the side reflector, where the leakage out of the core adds a directional dependence to the flux, further complicates the problem. One of these methods is the Method of Equivalent Cross Sections, which was proposed by Scherer and Fen [33]. The principle is to model the absorber and its environment in transport theory ($S_N$) and then extract cross sections and diffusion parameters from the transport solution that will represent the absorber region accurately in subsequent 3-D diffusion calculations.

Another very simplified method available, called the Equivalent Boron Concentration (EBC), consists of adding a certain amount of boron absorber homogeneously into a “borated region” representing the control rod. The concentration of the boron is adjusted so that the control rod worth is conserved. The method assumes that the rod reactivity worth is known from experiment or other methods such as MECS.

In this work the 3-D neutron transport $S_N$ code TORT [34], was used with the cross sections generated from MICROX-2 to perform control rod worth calculations with control rods accurately and explicitly modeled in three-dimensions. The task here is to first get the accurate control cross sections and to apply them in the neutronics code, whilst at the same time coming up with the best possible geometric representation of the
control rod in TORT. The main objective of these studies was to obtain an optimum control rod representation in TORT, and use the differential control rod worth curve resulting from this configuration to adjust the 2-D DORT-TD control rod approximation so that accurate transient analysis can be performed with the developed coupled-code DORT-TD-THERMIX. The approach used was to first evaluate the accuracy of the grey curtain representation of control rods by comparing it to MCNP and then proceed to develop an explicit 3-D model in TORT and MCNP.

### 6.1 Core and Control Rod Models Developed

In this study, three control rod models were developed and extensively evaluated for accuracy. The first one as mentioned above was the grey curtain representation. The grey curtain was used in DORT (r-z geometry) and also used in TORT (r-θ-z geometry) with a dummy theta dimension. This exercise was meant to verify TORT, because using the same cross sections and this dummy theta dimension, the TORT model is the same as the DORT model, hence one expects that the results obtained by the two codes should ideally be the same. This grey curtain model was also developed with MCNP, just for verification purposes. Secondly, an explicit model in MCNP was developed to represent Figure 6-1 the control rods explicitly i.e. not as a grey curtain. Thirdly, a TORT was developed and was made to be as close as possible to the MCNP to accurately model the control rod configuration of the PBMR 268MWt design. Before proceeding to the models themselves, it is important to first discuss the PBMR control design.
The control rods in the PBMR are located in holes in the side reflector. These “sleeves” are made of graphite and the control rod is an annulus of Boron carbide within a cladding, as shown in Figure 6.1 below:

![PBMR control rod design](image)

Figure 6-1: PBMR control rod design

There are 18 control rods and 17 shut down rods filled with small absorber sphere called KLAKS. For purposes of this study, the shut down elements were not modeled as these are not used during normal operation. Inner radius of control rod channel sleeve is 6.5 cm and the outer radius is 7.3 cm. In this study, the control rod can be inserted as far as 850 cm, which is the height of the active core. Again, in the actual PBMR design, control rods are divided into two sets, with 9 inserted from the bottom and 9 from the top,
thereby creating a possibility of control rod overlap. It assumed in this work that all rods are full length and thus they will overlap for the total height of 8.5m.

In both TORT and MCNP, the design data used was obtained from the PBMR Company in South Africa, and this is the same data the designers use for their models. Table 6 below, gives a summary of the dimensions of the control elements whilst number densities and material composition data is given in Table 6.1 and Table 6.2.

Table 6-1: Control Element Design Data

<table>
<thead>
<tr>
<th>Control Rod and KLAK Channels</th>
<th>Other info</th>
<th>Outer Radius (cm)</th>
<th>Thickness (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Control Rods</td>
<td>PCD</td>
<td>375 cm</td>
<td>-</td>
</tr>
<tr>
<td>Number of Control Rods</td>
<td>18</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Number of KLAK Channels</td>
<td>17</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Incoloy Inner Radius</td>
<td>4.1 cm</td>
<td>-</td>
<td>-</td>
</tr>
<tr>
<td>Control Rods</td>
<td>Inner Incoloy</td>
<td>-</td>
<td>4.2</td>
</tr>
<tr>
<td>B4C</td>
<td>-</td>
<td>5.05</td>
<td>0.85</td>
</tr>
<tr>
<td>Outer Incoloy</td>
<td>-</td>
<td>5.25</td>
<td>0.2</td>
</tr>
</tbody>
</table>
Table 6-2: Incoloy (Inc800H) Material Composition of Control Rods

<table>
<thead>
<tr>
<th>Nuclide</th>
<th>Weight Percentage</th>
</tr>
</thead>
<tbody>
<tr>
<td>C-nat</td>
<td>0.07</td>
</tr>
<tr>
<td>Si-nat</td>
<td>1.00</td>
</tr>
<tr>
<td>P-31</td>
<td>0.03</td>
</tr>
<tr>
<td>S-32</td>
<td>0.02</td>
</tr>
<tr>
<td>Cr-nat</td>
<td>21.00</td>
</tr>
<tr>
<td>Mn-55</td>
<td>1.50</td>
</tr>
<tr>
<td>Fe-nat</td>
<td>43.38</td>
</tr>
<tr>
<td>Co-59</td>
<td>1.00</td>
</tr>
<tr>
<td>Ni-nat</td>
<td>32.00</td>
</tr>
</tbody>
</table>

From the data above, the MCNP model was developed for Case N2 of the PBMR 268Mwth Benchmark problem as discussed in the introductory sections of this thesis. Since this case requires cross sections generated at 900K and MCNP can perform calculations at room temperatures, further cross section processing was performed with the NJOY code [35] so as to finally produce the cross section file xsdir for MCNP at 900K. As mentioned earlier, two MCNP models were developed, namely, MCNP-grey curtain and MCNP-explicit. These models are shown in Figure 6.2, Figure 6.3 and Figure 6.4 below.
Figure 6-2: Radial cut of the PBMR 268MWth MCNP Model – Grey Curtain CR

Figure 6-3: Axial cut of the PBMR 268MWth MCNP Model – Grey Curtain CR
In developing the TORT model of the PBMR, BOT3P, the preprocessor (and postprocessor) of DORT and TORT was used. This approach was chosen because it would eliminate the possibility of geometrical errors in the model. With BOT3P, the user can actually visualize the geometry of the model and one of the salient features of this tool is that it can make the necessary adjustment in case of simple mistakes like overlaps or mesh size. It also has features that ensure that the volume of the model is preserved in case of some approximations due to small mesh size. The resulting TORT model is shown in Figure 6.5 below.
6.2 Control Rod Worth Calculations and Results.

From the developed models above, core calculations were performed with a view of computing control rod worths for each model. Firstly, it was important to verify that with TORT and DORT, using the same cross sections and a dummy theta dimension in TORT, i.e., both using the grey curtain representation of the control region, the results will be the same as expected. Calculations were performed at various insertion depths of the grey curtain with steps of 100 cm. The results obtained are shown below.
In Figure 6.6 above the ratio of rod reactivity worth at a given insertion step to rod reactivity worth when rods are fully inserted is plotted against $x/H$ where $x$ is the insertion step or distance, and $H$ is the height of the active core, in this case 850 cm. From the figure, it is clear that as expected, TORT in two dimensions completely reproduced the DORT results. This helps to verify TORT for PBMR modeling, as there is no published literature that the author is aware of in this regard. The same calculations were performed with MCNP using the grey curtain representation of the control region. The results of MCNP were compared with those of DORT and TORT and as shown in Figure 6-7 below, other than the apparent deviation as the control rods are inserted deeper into the core, there is a reasonable agreement between the these results. The MCNP calculations were performed using MCNP5 with 10000 cycles with 100 inactive cycles and 5000 history/cycle. In both DORT and TORT the convergence criteria used for the eigenvalue ($k_{eff}$) is $10^{-6}$. 
Since there was a reasonable agreement between the codes whilst using the grey curtain model of control rod representation, further calculations were performed with MCNP but this time, using the explicit model of control rods. The results were compared to the MCNP results with the grey curtain, to evaluate the accuracy of the grey curtain representation. The results show some differences on the control rod worth between these two models, but the overall result is reasonable agreement.
The objective of performing these calculations is to finally benchmark the DORT-TD code for PBMR and to later couple it with THERMIX-DIREKT. The coupled code will be used for transient analysis and one of the envisaged transient cases to be modeled with the coupled code is the rod ejection incident. It is therefore important that DORT-TD can model rod worth calculations accurately. In two-dimensions, the only feasible way to model control rods is by means of a grey curtain approximation. For this reason, rod worth calculations from DORT-TD are compared with MCNP explicit model below.

Figure 6-8: Control rod worth results – evaluating the accuracy of the grey-curtain representation
Figure 6-9: Control rod worth results – evaluating the accuracy of the DORT-TD grey-curtain model.

It can be concluded from the figure above, that the grey-curtain model in DORT-TD agrees excellent with the results of MCNP using explicit representation of control rods in the PBMR 268MWth design.

So far, all the results presented above have been obtained from symmetric rod movement, i.e. it is assumed that the whole bank of control rods is moved. It is also important to model an asymmetric movement of control rods and to be able to do that, a three-dimensional deterministic model is necessary. The TORT model presented in Figure 15 was utilized for this purpose. Using the Equivalent Boron Concentration method, calculations were initially performed with MCNP (explicit model) with all control rods inserted in the core and the resulting eigenvalue was noted. Subsequently, an iterative series of calculations was performed between MICROX, GIP and TORT, the
goal being to find an eigenvalue in TORT which is reasonably close to the MCNP value.

The Boron number density in MICROX was adjusted accordingly and cross sections were generated and arranged into a format readable by GIP. GIP was used to process the cross sections into the FIDO format used by TORT and core calculations were then performed in TORT. This process was repeated until the target k-eff value was obtained in TORT. With the final cross sections obtained, the calculation is repeated with all rods withdrawn and the comparison between TORT and MCNP yielded good agreement.

Finally, a series of calculations in both TORT and MCNP was performed where, a single rod and subsequently a combination of rods in an asymmetric arrangement were inserted whilst the rest were fully withdrawn and the corresponding reactivity worth was calculated. The results are shown in Table 6.3 and Figure 6.10 below.

<table>
<thead>
<tr>
<th>Combination</th>
<th>MCNP (dk/k)</th>
<th>TORT (dk/k)</th>
<th>% Difference</th>
</tr>
</thead>
<tbody>
<tr>
<td>CR1+CR4+CR7</td>
<td>-0.022</td>
<td>-0.022</td>
<td>-2.20 (+47 pcm)</td>
</tr>
<tr>
<td>CR1+CR5+CR11</td>
<td>-0.028</td>
<td>-0.024</td>
<td>-0.03 (0 pcm)</td>
</tr>
<tr>
<td>CR1+CR10</td>
<td>-0.016</td>
<td>-0.016</td>
<td>-2.63 (+43 pcm)</td>
</tr>
<tr>
<td>CR1+CR13+CR17</td>
<td>-0.021</td>
<td>-0.021</td>
<td>0.22 (-5 pcm)</td>
</tr>
</tbody>
</table>
6.3 Summary

In this chapter, three-dimensional models of the PBMR 268MWth design were developed using the TORT and MCNP codes in order to evaluate the three-dimensional transport effects in this design. Control rod worths evaluation was used as an example of such 3-D effect and deterministic transport methods were employed to model this effect. Different methods were used to model the control rods in the PBMR, the grey-curtain and the explicit models. The results have shown that a good level of accuracy can be obtained using these deterministic methods because they compare very well with the reference.
MCNP results, provided that the equivalent cross sections are accurately calculated and applied in the deterministic code.
CHAPTER 7

COUPLING OF THE TIME-DEPENDENT TRANSPORT CODE TO THERMALHYDRAULICS

7.1 Introduction

Space-time effects in the dynamics of nuclear reactors must be considered within the framework of a full three-dimensional (3D) treatment of both neutron kinetics and thermal hydraulics. To achieve this goal, it has become a tradition nowadays to incorporate three-dimensional neutronics core simulators into system codes, the well known examples being RELAP and ATHLET [36]. The benefit of such development is to provide best-estimate simulation of transient scenarios with coupled core-plant interactions, making the use of simplified and conservative methods such as point kinetics, superfluous [37]. Most of such coupled-code systems as mentioned above make use of the diffusion approximation to solve the neutron transport equation, using fine or coarse mesh approximation, and few energy groups. Although diffusion theory model of neutron transport has played a crucial role in reactor theory; it has a number of widely documented and well known shortcomings. These shortcomings can partly be resolved by among other things, improving the treatment of the spatial variable, using more energy groups and most importantly, applying neutron transport theory methods. This is particularly important for novel concepts and designs of Generation IV systems for which little operation and experimental experience exists. It is thus desirable and important to
deploy the more accurate but also more expensive multi-group transport approach as part of a coupled code system, which is the subject of this work.

In this chapter, the calculational tools that have been used to develop the coupling between time-dependent transport theory-based code and thermal hydraulics are discussed. Three individual computers codes make up the developed coupled code system namely:

a) MICROX-2: creation of a cross section library
b) THERMIX- DIREKT: calculation of the reactor core thermal-hydraulics
c) DORT-TD: calculation of the reactor core neutronics

In the following sections, the codes will be discussed in more detail. The last section will describe the methodology used in coupling of the codes. Additional improvements introduced in the codes as necessitated by the nature of the problem solved will also be discussed.

7.2 Description of the MICROX-2 cross section generation process

Most of the calculations performed in this study utilize cross sections generated by the MICROX-2 software package. This package consists of NJOY [35], MICROR [38] and MICROX-2, the three codes that were used in the cross section generation of the PBMR. NJOY is a nuclear data processing code that processes the evaluated nuclear data and produces the pointwise and multigroup cross sections. For this work, the processing of the ENDF-B/VI files is done using the 193 energy group structure, typical for thermal
high temperature gas-cooled reactors. The fast energy range consists of 92 groups while the thermal group energy range consists of 101 groups. MICROR is a reformatting module. It reformats the pointwise and multigroup (group wise) cross sections from NJOY and produces three output files: FDTAPE, GARTAPE and GGTAPE.

MICROX-2 is a one-dimensional two-region lattice cell code which uses integral transport theory method. It uses the three output files from MICROR to produce broad group cross sections for use in diffusion and transport codes. It solves the B1 neutron balance equations in a one-dimensional two-region unit cell and obtains the neutron weighting spectrum. The two regions are coupled by collision probabilities based on a spatially flat neutron emission (not flat neutron flux). The one-dimensional cell calculations are corrected for multi-dimensional lattice effects through Dancoff factors and bucklings. The code can process up to 11 mixtures and a maximum of 13 fission spectra for each spatial region. It has three geometry options: spherical, cylindrical and planar (slab).

In spherical geometry, the inner region of the unit cell contains fuel particles (also called kernels or grains). The code has the capability of treating two types of grains in this region. The outer region consists of the shell, moderator and coolant. For the spherical geometry as in the case of the pebble fuel, the two regions of the pebble cell are distinguished as follows: Region 1 consists of the inner fuel region. This is the 5-cm diameter region that contains the fuel kernels in the graphite matrix. The graphite shell and the moderator/coolant regions are homogenized into one region to make Region 2 as illustrated in Figure 7.1.
The group structure in MICROX-2 is such that the thermal energy cutoff is at 2.38 eV. For the 193 energy group structure, the maximum energy is $1.49 \times 10^7$ eV. MICROX-2 allows a fission spectra combination of up to thirteen fissionable isotopes. The user-specified fission spectrum weights are used to normalize the space and energy integral of the spectra. Isotropy is assumed for the fission contributions to the fine group sources. The treatment of the unresolved resonances relies on the interpolation of dilution-dependent fine group data and the pointwise data in the unresolved resonance energy range that is covered by the pointwise resonance calculation in the MICROR module.
MICROX-2 has options to output cross sections for both diffusion and transport theory codes, utilizing the output files NDUNIT and NTUNIT respectively. This feature came in very handy for this work because the purpose was to perform calculations in both diffusion and transport theory methods. For use in the transport code DORT-TD, further processing of the cross sections was required using the GIP code which basically reformats the cross sections from MICROX-2 to a format readable by DORT-TD. Finally, the reformatted cross sections are then packed into cross section libraries in the form of multi-dimensional tables using a simple Visual Basic script. Figure 7.2 illustrates the connection and flow of data from one code to the other as used in this study.

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**Figure 7-2: Cross section generation process in the MICROX-2 package**
7.3 Description of the THERMIX-DIREKT computer code.

The thermal hydraulic computer code THERMIX was developed at the Institute for Reactor Development, which is now known as ISR in Juelich, Germany. The code consists of two large sub-programs called THERMIX (heat conduction and heat radiation) and KONVEK (quasi-steady-state gas flow and quasi-steady heat transfer in regions where flow occurs). The code was designed to simulate steady-state operation, operational transients, as well as slow accident transients in high-temperature reactor. The code is also suitable for recalculating the results of natural convection experiments, which were carried out in pebble beds. When natural convention processes in the primary cycle were investigated, it was found that the iterative single-step method that had been used to calculate gas flow was no longer suitable. If this iterative method is used for the areas that are formed during natural convection in empty spaces where flow is more or less stagnant, insufficient convergence or even no convergence is obtained. This lead to further development of the convection module of the code and hence the code had to be partly re-written and the name changed to THERMIX-DIREKT. This code was designed for the calculation of two-dimensional problems. Basically the models used in this code are calculated in terms of cylindrical geometry, i.e. a mesh is superimposed in the r- and z-directions. The influence of angles (azimuthal) is not taken into account. The heat conduction and radiation component is also capable of calculating r-z-mesh using cylinder coordinates or x-y-meshes with Cartesian coordinates if the third dimension is ignored. The convection component has only been designed to simulate matrix grids in the r- and z-
directions. The computer model is divided into two different regions, which are called “compositions” and can be described as follows:

a) the solid model (THERMIX), a region which has the same material composition (material values, temperature-dependent heat conduction equations, temperature-dependent heat capacity equations),

b) the fluid model (DIREKT), a region in which the same hydraulic properties (percentage empty spaces/voids, hydraulic diameter), or the same type of internal geometry (e.g. pebble-bed, pipe geometry, or two-dimensional voids in which flow occurs), are present.

A mesh system is superimposed on this system of inter-connected “compositions”. Therefore every “composition”, consists of many or few material meshes depending on the degree of accuracy that is required. Within such a mesh, constant mean values apply to all the parameters. In the fluid model flow generally occurs in the r- and the z-direction in the “compositions” (with the exception of the solid region where no flow occurs). In the “compositions” which define pipes in which flow occurs in only one direction (e.g. the top and bottom reflectors) or one-dimensional circular areas, flow is only described in the z-direction. In the solid calculational model, heat conduction and thermal radiation are treated in a similar fashion. Inside the pebble-bed, heat transport which is due to heat conduction through the pebble and the coolant gas between the spheres plus the superimposed thermal radiation exchange between the sphere surfaces is described by a temperature-dependent effective heat conductivity equation with temperature dependent material constants as shown by Equation 7.1 below:
\[ \rho_s(T)C_s(T) \frac{\partial T}{\partial t} = \nabla(\lambda_s(T)\nabla T) + q_n'' + q_c'' \quad 7.1 \]

Where

\( \rho_s(T) \) is the solid structure density

\( C_s(T) \) is the heat capacity at temperature \( T \)

\( \lambda_s(T) \) is the effective conductivity which consists of contributions in conductivity

by the fluid, the solid structure and by radiation.

\( q_n'' \) and \( q_c'' \) are the possible volumetric heat sources in a mesh volume for nuclear and convective contribution respectively.

In \( r-z \) cylindrical coordinates, Equation 7.1 can be transformed after multiplication with the volume element into a model equation which can be solved numerically:

\[ \rho_s C_s \frac{\partial T}{\partial t} dV = d(\lambda_s \frac{\partial T}{\partial \ln r})2\pi dz + d(\lambda_s \frac{\partial T}{\partial z})2\pi dr + (q_n'' + q_c'')dV \quad 7.2 \]

It must be noted that only one temperature \( T \) occurs in this homogenized solids model with which the conductive and radiative thermal balance is calculated. This assumption is only valid if the heat production in the solid and hence the temperature differences in the fuel element are sufficiently small. For transients that involve scramming the reactor, this is possible because of the low decay heat production in the fuel element and its good heat conductivity. This does not apply to the calculation of power transients which occur under forced convection conditions. For such a scenario, the heterogeneous solids
temperature option of the THERMIX-DIREKT model has to be used. An improved
treatment of the temperature in order to account for the drawbacks of the homogeneous
treatment assumption was also introduced in the code as part of this work and will be
discussed later in the chapter.

The DIREKT module was developed in order to solve the time-dependent
equations for convection and to establish the gas temperature distribution for the reactor.
As such, it can be seen as the complimentary calculation to THERMIX to describe the fluid
part of a mesh volume. The heat convection calculation allows cross element heat transfer
in order to describe the circulation and eddying of the gas in the pebble-bed transient cases
with a halted mass flow rate. The first step towards obtaining the gas temperature
distribution is taken by combining the equations of continuity and motion, which yields the
pressure and mass flow rate distribution over the reactor at fluid temperatures of the
previous iteration. The second step consists of solving the energy equation with the new
pressure and mass flow rate distribution and solid temperature distribution from
THERMIX as input in order to determine the new gas temperature distribution. By iteration
over the two steps, convergence is reached in the solutions. When the new gas temperature
distribution is known, the convective source $q_c$ needed in THERMIX can be made explicit
by using Newton’s law of cooling:

$$q_c = \alpha A (T - T_g)$$  \hspace{1cm} (7.3)

The parameter $T_g$ is the gas temperature at which the heat transfer coefficient is
defined, and $A$ is the surface heat.
7.4 Description of the time-dependent transport code DORT-TD

DORT-TD, a numerically optimized transient extension of the well known steady-state SN code DORT, was developed at the Technical University of Munich, Germany in 2001. In developing the time-dependent features of DORT-TD, the usage of a fully implicit time discretization scheme was favored, which required the extension of DORT’s steady-state formulation by a “time-like” source term, precursor contributions and some modifications to total cross section and fission spectra. It is possible e.g. to take into account delayed neutron spectra different from the prompt fission spectrum as well as to have spatially varying neutron group velocities.

Outer iterations are accelerated through a number of different options. One such option is the widespread method of error mode extrapolation. This method is quite effective in the sense that if the error decay in the outer iterations assumes an asymptotic behaviour, a reasonable estimate of the so-called dominance ratio (i.e. the ratio of the two largest core eigenvalues) can be given. However, in some configurations and in particular for high accuracies (beyond $10^{-5}$, asymptotic error decay may be hard to achieve.

Another acceleration scheme to improve the convergence rate of the outer iterations, the so-called upscatter cycle is also present in DORT-TD. It is well known that in both steady-state and transient calculations, the iterative error decay often assume an asymptotic behaviour after a few outer iterations. However, this error decay can only be guaranteed if the inversion of the transport operators for each energy group were exact, i.e. the inner iterations were well converged. While this is normally easily achieved for fast groups by simply doing enough inner iterations, upscattering is known to pose
problems in the standard DORT version. This is because thermal groups in DORT are treated the same way as fast groups, i.e. they are only solved once per outer iteration. To partially account for upscatter, DORT uses the method of “upscatter rebalance”[34]. However this scheme has not been successful for systems with spatially inhomogeneous thermal spectrum. Against this background, this ineffective upscatter rebalance scheme in DORT was replaced by an “upscatter “cycle” in DORT-TD. Instead of inverting the group transport operator only once per energy group and per outer iteration, a loop over all thermal groups is executed within one outer iteration. This ensures that all groups receiving upscatter are properly converged.

To further enhance the convergence properties of the code, advantage was taken from the use of the Chebyshev polynomial method to perform a fission density extrapolation. The corresponding routine can optionally replace the error mode extrapolation, as it is implemented in standard DORT. The effectiveness of the Chebyshev scheme depends strongly on the so called dominance ratio of the system under consideration, i.e. the ratio of the two largest eigenvalues.

Another important feature of the DORT-TD code is that as a further enhancement of accelerating inner and outer iterations, one can benefit from the fact, that the solution of time-step n is in general quite a good approximation (unless time steps are too large) to the fluxes to be calculated at timestep n+1, and can be used as an excellent starting guess for the iterative scheme. This guess may still be improved by doing a time-like extrapolation. By constructing “reactor periods” from timestep n-1 and n, which are resolved in space as well as in angle and energy:
\[
\omega^{(n)}(r, \Omega, E, t_n) = \frac{1}{\Delta t} \ln \left( \frac{\psi^{(n)}(r, \Omega, E, t_n)}{\psi^{(n-1)}(r, \Omega, E, t_{n-1})} \right) 
\]

7.4

one can construct estimates for the angular fluxes \( \psi^{(n+1)} \):

\[
\tilde{\psi}^{(n+1)} = \psi^{(n)} \cdot \exp(\omega^{(n)} \Delta t_{n+1})
\]

7.5

Despite its simplicity, this scheme has proven to be quite effective. The use of the above mentioned Chebyshev acceleration, upscatter cycle and time-like extrapolation methods within the transient code system reduces the computing time needed for a single time step by more than an order of magnitude compared to the steady–state problem, although the numerical effort is formally the same [31]. This makes the use of the time-dependent transport code quite attractive, even when compared to quasistatic approaches.

**7.5 Description of the temporal and spatial coupling scheme**

In the following subsections, the general description of the coupling methodology as well as both the temporal and spatial coupling scheme is described.

**7.5.1 General Description**

The coupling is made up of three important components as shown in Figure 7.3.: 

1. The neutron kinetics part (DORT-TD or diffusion)
2. The thermal hydraulics part (THERMIX-DIREKT)
3. The cross section interpolation performing at each time-step the calculation of the cross sections corresponding to the thermal hydraulic state of the system
In the coupling scheme, a feedback model was developed to account for the neutronics feedback effects and implemented into DORT-TD. The feedback parameters of interest in the model are fuel temperature \( (T_f) \), moderator temperature \( (T_m) \), and Xenon feedback. This model can also be extended to include other feedback parameters such as burnup and spectrum/leakage feedback. Two routines have been developed as part of this feedback model. The first routine automatically generates a macroscopic cross section library for a given PBMR core model using the cross section generation code MICROX-2. This library contains sets of macroscopic cross section tables for up to 5-D dimensions for each composition. Users can specify the ranges of the feedback parameters as well as the number of reference points themselves. This library contains tables for transport, total transport-corrected, absorption, fission, production and scattering cross sections. The second routine reads the tables and interpolates in them to obtain the microscopic cross section values for each spectral zone (core region) and for each broad energy group. The interpolation routine uses tensorial products of one dimensional B-splines of arbitrary order, and was taken from the DB3INK routine of the CMLIB library [46].
As shown in Figure 7-3, any transient analyses starts with a criticality search. At the very beginning the pre-calculated nuclear cross section files are transferred to memory. With an approximate user-supplied power profile THERMIX can compute a first estimate of local temperature and density distributions in the reactor core. From these thermal hydraulic parameters, local multigroup cross sections are generated by interpolation from the cross section library. Using these cross sections, a first transport calculation is performed, resulting in a $k_{eff}$, which will most likely not be equal to unity. After adjusting e.g. control rod positions, a new iteration between THERMIX and
neutron kinetics can be started. This loop is carried out until thermal hydraulics system parameters and neutron fluxes, power densities as well as the effective multiplication factor are sufficiently converged. In this starting phase it is possible to achieve a $k_{\text{eff}}$, which is converged as close as $10^{-8}$ to unity, corresponding to reactor periods of several years.

At this stage, an arbitrary transient can be initiated, e.g. control rod ejection, depressurization etc. When this happens, the code first perform a so called “zero transient” for a certain time to assure that under steady-state conditions the system remains in global balance before the “real” transient is started. The code system provides for an eventual change of material composition or geometry during a transient, which can be done at the beginning of any time step. Through this, one can e.g. achieve a continuous movement of control rods or other geometrical structures. After that, the thermal hydraulics data are received from the THERMIX calculation and new cross sections are generated. The updated macroscopic cross sections are passed back to DORT-TD to perform transport core calculations, and the power distribution is transferred to THERMIX-DIREKT in order to compute the new system state, and a new time step can be started, and this calculation loop continues until the transient is terminated.

7.5.2 Spatial Coupling Arrangement

In order to establish a seamless exchange of data spatially, there are four superimposed meshes in the scheme, namely: neutronics, thermal hydraulics, feedback and power
density meshes. The thermal hydraulics mesh (THERMIX-DIREKT) has the largest spatial extent such that all other meshes fall inside this mesh. Each thermal hydraulics mesh line inside the neutronics region must correspond to the neutronics mesh lines. The feedback mesh must always be the subset of the neutronics mesh. The power density mesh must always be the subset of the neutronics mesh and the thermal-hydraulics mesh. If these requirements are not fulfilled, the code terminates. Currently, it is not possible to interpolate mesh values if the meshes do not coincide according to the above rules. This could be a future improvement of the code which will allow for more flexibility and simpler input preparation. This spatial coupling arrangement is illustrated in Figure 7.4 below.

Figure 7-4: Spatial mesh overlay in the DORT-TD/THERMIX coupling

As can be seen in Figure 7-4, the neutronics mesh is superimposed on the thermal hydraulics mesh, only to the extent where the reflectors are located. Then the so-called feedback mesh lies over both the neutronics and thermal hydraulics meshes, essentially coarser than the neutronics mesh (in principle however, it could be as fine as the thermal-
hydraulics mesh). In this sense, thermal-hydraulic feedback parameters (i.e. the moderator and the Doppler temperatures etc.) are treated as an average over at least one or a larger set of thermal-hydraulics nodes and projected into the feedback mesh. From these feedback values, for each mesh point of the feedback mesh, cross sections are generated and then projected back to neutronics mesh, via the cross section data base.

### 7.5.3 Temporal Coupling Scheme

The temporal coupling is driven by THERMIX-DIREKT. During a given transient, THERMIX-DIREKT sets the time-step, which will always be larger than DORT-TD’s. To control and limit this time-step in the neutronics, DORT-TD imposes a rough and reasonably conservative estimate of the numerical truncation error. This is done by considering a truncation error of simple exponential which is then compared to the solution of the transport equation. To illustrate this, consider the following differential equation and its fully implicit formulation:

\[
\frac{\partial^n \Psi}{\partial t^n} = \omega^n \Psi \rightarrow \frac{\Psi^{(n+1)} - \Psi^{(n)}}{\Delta t_n} = \omega^n \Psi^{(n+1)}
\] 7.6

The solution to both equations and the corresponding series expansions are:

\[
\Psi(t + \Delta t) = \Psi(t) \exp(\omega \Delta t)
\]

\[
\approx \Psi(t) \left(1 + \omega \Delta t + \frac{1}{2!} \omega^2 \Delta t^2 + O(\Delta t^3) \right)
\]

\[
\Psi^{(n+1)} = \Psi^{(n)} \frac{1}{1 - \omega \Delta t_n}
\]

\[
\approx \Psi^{(n)} \left(1 + \omega \Delta t_n + \omega^2 \Delta t_n^2 + O(\Delta t_n^3) \right)
\] 7.7
The truncation error $\tau$ of the implicit scheme after $N$ time steps is thus given by:

$$\tau = |\Psi(t)| \frac{1}{2} N \omega^2 \Delta t^2 O(\Delta t^2)$$  \hspace{1cm} 7.8

For an absolute transient length of $T = N \Delta t$ and a user prescribed relative error $\tau_{rel}$, one can derive an expression for the maximum length of the subsequent time-step:

$$\Delta t_{\text{max}} = \frac{2\tau_{rel}}{\omega^2 T}$$  \hspace{1cm} 7.9

For $\omega$ (the reactor period), a maximum value of the phase-space inverse resolved reactor period is chosen in DORT-TD using the expression:

$$\omega^n (r, \Omega, E) = \frac{1}{\Delta t_{n-1}} \ln \left( \frac{\Psi^{(n)} (r, \Omega, E)}{\Psi^{(n-1)} (r, \Omega, E)} \right)$$  \hspace{1cm} 7.10

It may also be helpful to reduce the time-step predicted by Equation 7.10 by some prescribed value (e.g. 1.2) to improve the convergence rate of the outer iteration cycle if a certain number of outer iterations (10 to 15) is exceeded.

The evaluation of the time step size described is performed at the outset of each time step. If after this evaluation, the THERMIX-DIREKT time-step size is far too large for DORT-TD, DORT-TD subdivides this time-step into several smaller time-steps, such that the last time-step for that interval is synchronized with the THERMIX-DIREKT time-step, and hence data is only exchanged at the first and last time-points as illustrated in Figure 7-5 below:
Figure 7-5: DORT-TD/THERMIX timestep control

With the above temporal arrangement, the code yields well converged solutions. Typically, the convergence criteria satisfied by the code is thus:

(a) Eigenvalue (steady-state) or overall reaction rate balance (time dependent) convergence: \( \varepsilon = 5 \times 10^{-9} - 10^{-7} \)

(b) Pointwise flux convergence: \( \varepsilon = 5 \times 10^{-7} - 10^{-6} \)

These values are highly recommended for most types of time-dependent applications and have turned out to be mainly sufficient. Setting less restrictive error conditions may lead to erroneous results.
CHAPTER 8
VERIFICATION AND VALIDATION OF THE COUPLED CODE DORT-TD/THERMIX

8.1 Introduction

In the previous chapter, a lot of attention was given to the various components that make up the coupled neutron transport-thermal-hydraulic code DORT-TD/THERMIX. In any code development process it is always important to subject the developed code to rigorous verification and validation exercises. For purposes of this work, verification is defined as the process determining whether or not the program is coded correctly and conforms to the specified requirements. An acceptable verification method is to develop a series of calculation cases or input decks that test much of the logic in the code to ensure that the code performs as stated in the theory. On the other hand, validation is defined as the process of evaluating the code to ensure compliance with physical applicability to the process. It would consist of comparing the code with known analytical solutions or against an already validated computer code, or better still, benchmarking the code against relevant experimental data.

Unfortunately, for new designs that are still under review such as the PBMR, not much experimental data exists to benchmark newly developed computer codes against. In such a situation, it is reasonable to resort to the validation of a newly developed code through a code to code benchmarking exercise because there are validated codes that are currently in use to analyze this reactor design, albeit very few of them. There are numerous HTR core physics benchmarks that are currently being pursued by different
organizations, for different purposes. One such benchmark exercise which is more relevant to the objectives of this work is the PBMR-400 OECD/NEA coupled neutronics/thermal hydraulics transient benchmark and will be described in the next section.

This chapter is divided into two main sections, the first one being the validation of the DORT-TD/THERMIX coupled code using the PBMR 400 OECD/NEA benchmark. The second section will focus on the verification of DORT-TD/THERMIX’s higher order transport capability in analyzing two-dimensional transport effects during transients, using the PBMR 268MW design described earlier in Chapter 5. The results of these two main activities will be presented and discussed.

8.2 The PBMR-400 OECD/NEA coupled neutronics/thermal hydraulics transient benchmark

Over the years, different organizations have emerged with numerous benchmark problem definitions and experimental facilities for high-temperature reactors, including a few existing for pebble-bed reactors. This includes, amongst others, the HTR-Proteus pebble-bed critical experiments at the Paul Scherer Institute in Switzerland and the ASTRA facility at the Research Centre Kurchatov in Russia as examples of critical assemblies. Then there is an HTR-10 reactor in operation at Tsinghua University, Beijing, China, and the reactors that operated in Germany in the past such as the AVR, and finally, several code-to-code comparisons performed as part of the IAEA CRP-5 project on “Evaluation of HTGR Performance”. All of these contributed to the
benchmarking and verification and validation of coupled neutronics/core thermal-hydraulics tools used in pebble-bed reactor designs.

The focus of the PBMR 400 OECD benchmark test cases is on developing coupled kinetics-core thermal-hydraulics test problems that include both fast (reactivity insertions) and slow (thermal heat up due to decay heat) transients. The reference design for this benchmark problem is derived from the PBMR 400MW design shown in Figure 8.1 below.

![Figure 8-1: PBMR 400 Reactor Unit](image)

The design is an annular core with an outer diameter of 3.7 m and a ‘fixed central reflector’ with an outer diameter of 2 m, an effective cylindrical core height of 11 m and a
An graphite side reflector of 0.9 m. The Reactivity Control System (RCS) consisting of 24 partial length control rod positions is situated in the side reflector, with 12 upper or control rods and 12 lower or shutdown rods when fully inserted. During normal operation all 24 rods operate together. The rods have an effective length (B₄C neutron absorbing material) of 6.5 m. In addition, the Reserve Shutdown System (RSS) consisting of eight Small Absorber Sphere (SAS) systems is positioned in the fixed central reflector and filled with 1 cm diameter absorber spheres containing B₄C when required. Three fuel loading positions and three fuel unloading tubes are positioned equidistant in the centre of the fuel annulus. The core contains ~ 452,000 fuel spheres or “pebbles” with a packing fraction of 0.61. The uranium loading is 9 g per fuel-sphere with the U²³⁵ enrichment at 9.6 wt%. The inner 5 cm of the fuel sphere contains about 15 000 UO₂ TRISO-coated micro-spheres within a graphite matrix and surrounded by an outer graphite fuel free zone. Each coated particle acts as a fission product barrier [39].

The fuelling scheme employed is the continuous on-line multi-pass method similar to the designs used in Germany. Fresh fuel elements are added to the top of the reactor while used fuel pebbles are removed at the bottom to keep the reactor at full power. On average, each fuel pebble makes six passes, through the reactor before being finally discharged to the spent fuel storage tanks with a target burn-up of >90,000 MWd/tU.

Other design and operating characteristics of interest in this design are presented in Table 8.1.
Table 8-1: Major Design and Operating Characteristics of the PBMR

<table>
<thead>
<tr>
<th>PBMR Characteristic</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Installed thermal capacity</td>
<td>400 MW(t)</td>
</tr>
<tr>
<td>Installed electric capacity</td>
<td>165MW(e)</td>
</tr>
<tr>
<td>Load following capability</td>
<td>100-40-100%</td>
</tr>
<tr>
<td>Availability</td>
<td>≥ 95%</td>
</tr>
<tr>
<td>Core configuration</td>
<td>Vertical with fixed centre graphite reflector</td>
</tr>
<tr>
<td>Fuel</td>
<td>TRISO ceramic coated U-235 in graphite spheres</td>
</tr>
<tr>
<td>Primary coolant</td>
<td>Helium</td>
</tr>
<tr>
<td>Primary coolant pressure</td>
<td>9Mpa</td>
</tr>
<tr>
<td>Moderator</td>
<td>Graphite</td>
</tr>
<tr>
<td>Core outlet temperature</td>
<td>900°C.</td>
</tr>
<tr>
<td>Core inlet temperature</td>
<td>500°C.</td>
</tr>
<tr>
<td>Cycle type</td>
<td>Direct</td>
</tr>
<tr>
<td>Number of circuits</td>
<td>1</td>
</tr>
<tr>
<td>Cycle efficiency</td>
<td>≥ 41%</td>
</tr>
<tr>
<td>Emergency planning zone</td>
<td>400 meters</td>
</tr>
</tbody>
</table>

In order to enable as many participants in the benchmark as possible without major code changes to their existing codes, several simplifications were made to the design specification so that the need for any further approximations is limited. Furthermore, multi-dimensional cross-section library and interpolation routines are supplied to participants as the basis for all transient studies. This would eliminate differences due to different sources of cross-section data and preparation.

During the simplification process, care has been taken to ensure that all the important characteristics of the reactor design are preserved. The simplifications make the core design essentially two-dimensional (r, z). Flow channels within the pebble bed have been simplified to be parallel and at equal speed while the dynamic central column
and mixing zone widths were defined to be constant over the total axial height. This implies flattening of the pebble-bed's upper surface and the removal of the bottom cone and de-fuel channel that results in a flat bottom reflector. Control rods in the side reflector are modeled as a cylindrical skirt (also referred to as a grey curtain) with a given B10 concentration. A multi-pass fuel circulation (MEDUL with 10 passes) and vertical pebble flow are assumed.

Thermal-hydraulic simplifications include the specification of stagnant helium between the barrel and reactor pressure vessel (RPV) and stagnant air between the RPV and heat sink (outer boundary). The coolant flow is restricted to upwards flow from the inlet below the core within a porous ring in the reflector and downwards flow through the pebble bed to the outlet plenum. No reflector cooling or leakage paths were defined.

Other simplifications include the assumption that all heat sources (from fission) will be deposited locally, i.e. in the fuel, and that no other heat sources exist outside the core (for example neutron absorption in the control rod region). Simplifications are also made in the material thermal properties, in as far as constant values are employed or specific correlations are employed. When all the simplifications have been made, the model of the reactor unit in Figure 8.1 is transformed to the model shown in Figure 8.2. Further details of the benchmark problem, material specifications, geometric description etc can be obtained in [40].
<table>
<thead>
<tr>
<th>Z</th>
<th>REACTOR CORE CONTAINING THE FUEL</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>CENTRAL REFLECTOR: GRAPHITE</td>
</tr>
<tr>
<td>50</td>
<td>TOP REFLECTOR: GRAPHITE</td>
</tr>
<tr>
<td>100</td>
<td>BOTTOM REFLECTOR: GRAPHITE</td>
</tr>
<tr>
<td>150</td>
<td>SIDE REFLECTOR: GRAPHITE</td>
</tr>
<tr>
<td>200</td>
<td>RESERVE SHUTDOWN SYSTEM CHANNEL: GRAPHITE / GREY CURTAIN AREA</td>
</tr>
<tr>
<td>250</td>
<td>INLET PLENUM TOP / BOTTOM: GRAPHITE</td>
</tr>
<tr>
<td>300</td>
<td>RISER CHANNEL IN SIDE REFLECTOR: GRAPHITE</td>
</tr>
<tr>
<td>350</td>
<td>OUTLET PLENUM BOTTOM: GRAPHITE</td>
</tr>
<tr>
<td>400</td>
<td>STAGNANT HELIUM</td>
</tr>
<tr>
<td>450</td>
<td>TOP PLATE: IRON : ADIABATIC BOUNDARY</td>
</tr>
<tr>
<td>500</td>
<td>BOTTOM PLATE: IRON : ADIABATIC BOUNDARY</td>
</tr>
<tr>
<td>550</td>
<td>CORE BARREL: IRON</td>
</tr>
<tr>
<td>600</td>
<td>REACTOR PRESSURE VESSEL: IRON</td>
</tr>
<tr>
<td>650</td>
<td>STAGNANT AIR</td>
</tr>
<tr>
<td>700</td>
<td>REACTOR CAVITY COOLING SYSTEM : 20C TH BOUNDARY</td>
</tr>
<tr>
<td>750</td>
<td>NEUTRONIC BOUNDARY BONDITIONS</td>
</tr>
</tbody>
</table>

**Figure 8-2: PBMR 400 Core Layout and material identification**
The benchmark prescribes several steady-state and transient cases using the cross section library supplied with the benchmark specification. For purpose of validating the DORT-TD/THERMIX code, the above model was developed and selected calculational cases were performed with the code as will be discussed in later sections.

8.3 Steady-state analysis of the PBMR-400 Benchmark

In this section, the steady-state problem is described together with the cross section library that will be used for both the steady-state and the transients. Results of DORT-TD/THERMIX will also be presented in general and will in the later sections be compared with other benchmark results in particular.

8.3.1 Description of the steady-state Exercise 3

The steady-state problem modeled here is referred to as Exercise 3 in the benchmark specification. This Exercise is the steady-state starting condition of all the transient cases. It makes use of state parameter dependent tabulated set of macroscopic cross sections. It is required that a coupled neutronics-thermal hydraulic calculation be done with feedback. Equilibrium xenon distribution, temperature distribution as well pressure drop over the core are to be calculated.
8.3.2 Description of the cross section data layout

Cross section interpolation routines were provided with the benchmark specification and were implemented in the code as well as the routine to read the tabulated cross section data library. In these two-energy group libraries, five-dimensional tables are used to represent the instantaneous variation in cross-section due to changes in the reactor. The cross section models are designed to cover the initial steady state conditions and the expected ranges of change of the five selected instantaneous feedback parameters in the transients to be simulated in the benchmark. Cross sections were generated for all the combinations of the given state parameters. The five state parameters are:

- Fuel temperature
- Moderator temperature
- Fast buckling
- Thermal buckling
- Xenon concentration

In all of the fuel material cross section tables, there were four fuel temperatures (300K, 800K, 1400K, 2400K), seven moderator temperatures (300K, 600K, 800K, 1100K, 1400K, 1800K, 2400K), three fast group bucklings, three thermal bucklings and three Xenon number densities while for all the non-fuel materials no fuel temperature or xenon variations are included. The ranges chosen for each parameter were selected based on the reactor conditions for normal operation as well as for accident conditions. Several code changes were required in DORT-TD in order to include the buckling as a feedback parameter in accordance with the benchmark specification. Buckling is defined as follow:
\[ \beta^2 = \frac{L}{D \phi V} \text{ [cm}^{-2}] \];

where \( \beta^2 \) is the Buckling; \( L \) is the total out leakage from a given mesh or region; \( D \) the diffusion coefficient; \( \phi \) the average flux and \( V \) the region volume. This was implemented in DORT-TD and its effect in the results will be shown later.

With all the feedback parameters included in the cross section library, the parameter variation in the library during a given transient is given in Figure 8.3 below.

<table>
<thead>
<tr>
<th>( T_{f1} )</th>
<th>( T_{f2} )</th>
<th>( T_{f3} )</th>
<th>( T_{f4} )</th>
<th>( T_{m1} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T_{m2} )</td>
<td>( T_{m3} )</td>
<td>( T_{m4} )</td>
<td>( T_{m5} )</td>
<td>( T_{m6} )</td>
</tr>
<tr>
<td>( T_{m7} )</td>
<td>( B_{f1} )</td>
<td>( B_{f2} )</td>
<td>( B_{f3} )</td>
<td>( B_{f1} )</td>
</tr>
<tr>
<td>( B_{f1} )</td>
<td>( B_{f3} )</td>
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</table>

Figure 8-3: Key to macroscopic cross sections library

where:

- \( T_f \) is the fuel temperature
- \( T_m \) is the moderator temperature
- \( B_f \) is the fast buckling
- \( B_m \) is the thermal buckling
- \( X \) is the Xenon number density
- \( \Sigma \) is the macroscopic cross section

The layout of cross section tables is as follows:

- \( \Sigma_1 \) is a function of \((T_{f1}, T_{m1}, B_{f1}, B_{t1}, X_1)\)
- \( \Sigma_2 \) is a function of \((T_{f2}, T_{m1}, B_{f1}, B_{t1}, X_1)\)
- \( \Sigma_3 \) is a function of \((T_{f3}, T_{m1}, B_{f1}, B_{t1}, X_1)\)
- \( \Sigma_4 \) is a function of \((T_{f4}, T_{m1}, B_{f1}, B_{t1}, X_1)\)
• \( \Sigma_5 \) is a function of \((T_{f1}, T_{m2}, B_{f1}, B_{t1}, X_1)\)
• \( \Sigma_6 \) is a function of \((T_{f2}, T_{m2}, B_{f1}, B_{t1}, X_1)\)
• \( \Sigma_7 \) is a function of \((T_{f3}, T_{m2}, B_{f1}, B_{t1}, X_1)\)
• \( \Sigma_8 \) is a function of \((T_{f4}, T_{m2}, B_{f1}, B_{t1}, X_1)\)
• \( \Sigma_9 \) is a function of \((T_{f1}, T_{m3}, B_{f1}, B_{t1}, X_1)\)
• \( \Sigma_{10} \) is a function of \((T_{f2}, T_{m3}, B_{f1}, B_{t1}, X_1)\)
• ...
• \( \Sigma_{29} \) is a function of \((T_{f1}, T_{m1}, B_{f2}, B_{t1}, X_1)\)
• ...
• \( \Sigma_{85} \) is a function of \((T_{f1}, T_{m1}, B_{f1}, B_{t2}, X_1)\)
• ...
• \( \Sigma_{253} \) is a function of \((T_{f1}, T_{m1}, B_{f1}, B_{t1}, X_2)\)
• ...
• \( \Sigma_{756} \) is a function of \((T_{f4}, T_{m7}, B_{f3}, B_{t3}, X_3)\)

Finally, the cross section table with the range of all variables is shown in Table 8.2. The total macroscopic absorption cross-sections provided exclude the absorption effect of xenon that should be treated explicitly by the core analysis codes. In order to make this possible, the xenon absorption was subtracted from the total cross section using the xenon microscopic cross sections and the input xenon number densities. The \( \beta \)s (delayed neutron fractions) and \( \kappa \) (energy release per fission) values are given per material per energy group while lambdas (precursor decay constants) are fixed values for each of the six precursor groups.
Table 8-2: Cross Section Table with a range of variables

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### 8.3.3 Results of Exercise 3 Using DORT-TD/THERMIX

In this section, the steady-state results of Exercise 3 of the benchmark are shown with the view of confirming the functionality and applicability of DORT-TD/THERMIX to this kind of a reactor, i.e. for code verification purpose. The code uses both diffusion and transport theory options but the results shown below are from the transport solution.

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</table>

Figure 8-4: 2-D Power Density Distribution from the top to the bottom of the core
From looking at the neutron thermalization process and interpreting the flux distributions, the figures above can be explained. The migration length for the neutrons is such that those neutrons born in the central core region are mostly thermalized by the graphite in the core. Neutrons further from the central core region are most likely to reach the side reflectors and are thermalized there virtually without loses (no parasitic absorption) compared to the thermalization in the fuel zone. The thermal flux distribution therefore has a local maximum in the central core region and an absolute maximum in the side reflector close to the reflector-core interface as seen in Figure 8.5. The reflector-
thermalized neutrons that return into the fuel zone diffuse only a short distance back into the core before being absorbed. This is reflected in the power density distribution which is proportional to the thermal flux in the core and has maxima in the core centre and along the side reflector as shown in Figure 8.4. The apparent wiggles in the power density curve in Figure 8.4 are as a result of the very fine mesh in DORT-TD which makes the discontinuities as one move from one burnup region to the other axially, more pronounced. It can be argued that in the fuel zone close to the side reflector, where fast fission neutrons are born, one would also expect a maximum for the fast flux. However, on average half the fast neutrons disappear into the reflector and are replaced by thermal neutrons, thus effectively halving the fast neutron density. This reasoning holds the same for top and bottom reflectors in the axial direction.

![Axial Power Density Profile](image)

Figure 8-6: Axial Power Density Distribution
The bottom reflector plays an important role mainly during the early stages of the core life. For a fresh core, the active part lies just above the bottom reflector and along the side reflector as there the thermal flux is maximal. As time progresses and fuel depletes, fresh fuel is added on top of the core. The most active part of the core then changes position and shifts from the bottom to the top region of the core. During subsequent core life, the active part of the remains in the top region of the core and slowly shifts up, as is the case with Exercise 3 under consideration here because an equilibrium core is assumed, hence the tendency for the power density to shift towards the top regions of the core in Figure 8.6.

The radial temperature distribution for the solid heat structures closely follows the radial power density distribution: regions with higher power density are hotter, i.e. the central core region and closer to the reflectors as shown in Figure 8.7. The coolant temperature distribution is a little smoother due to gas mixing with adjacent regions. The gas heats up while flowing from top to bottom through the pebble bed, and on exiting it streams through slits in the porous bottom reflector. In steady-state the bottom reflector experiences therefore a large temperature gradient as can be seen in Figure 8.8. At one side there is a coolant gas going through the central reflector hole, and on the other side the hot gas is exiting the reactor.
### Figure 8-7: Core Solid Structure Temperature Distribution

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### Figure 8-8: Helium Temperature Distribution in the Core Region

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Up to this point, the PBMR 400 MW benchmark Exercise 3 was used to illustrate the suitability of the DORT-TD/THERMIX coupled code in modeling this reactor design. In the results presented, it was shown that the code can model this problem, clearly reproducing known physics of the problem, leading to the conclusion that at steady-state conditions (as described by Exercise 3), the code can adequately handle the PBMR 400 core neutronics and thermal-hydraulics design characteristics, thus: DORT-TD/THERMIX has been verified for this design. Logically, the next step is to validate the code by modeling the same problem as other codes have modeled, and comparing the results. This is the subject of the next section.

8.4 DORT-TD/THERMIX coupled steady-state results versus other codes.

In the PBMR 400 benchmark problem, the steady state case (Exercise 3) is designed to initialize the participants’ models and to help understand better and reduce if possible the differences between participant results. This coupled steady state case also serve to test the coupling schemes of the codes and the associated feedback models. It also provides the starting conditions for all the transient cases, i.e. restart conditions. As was the case in the calculations of DORT-TD/THERMIX, all participants used the provided cross section tables with five dependent parameters thus: fuel and moderator temperatures, fast and thermal buckling and xenon density. Comparison of results was done for both thermal hydraulics and neutronics output but only the neutronics comparisons are presented here. Since the benchmark is still ongoing, only five participants from four countries had submitted their results at the time of writing this
thesis. Some outliers from the results were also deliberately excluded as some issue still needed to be sorted out with the participants’ models.

Figure 8-9: K-effective Comparison for Exercise 3

Table 8.9 above shows the comparison of $K_{\text{eff}}$ value between different codes compared to DORT-TD/THERMIX. It can be seen from the comparison that despite the spread in the results, DORT-TD/THERMIX is in excellent agreement with other codes. Since there is no real reference solution yet, it is difficult to judge which code is calculating the accurate results but other than one outlier, most participants are closer to each other and DORT-TD/THERMIX is amongst them. Moreover, the diffusion mode of the code is very close to the average value and this can be attributed to the full buckling feedback utilized in the diffusion module, whereas the transport module of the code only uses fixed buckling feedback, i.e. values obtained from the fully converged buckling
values from the diffusion mode of the code and hence the buckling value does not get updated later on during the transients. This is the current drawback of DORT-TD/THERMIX and this will be clearly observed when transient analysis studies are performed later in the chapter. Figures 8.10 and 8.11 shows comparison of the power densities whiles Figures 8-12 to 8-15 shows the comparison of thermal and fast fluxes averaged along both the radial and axial directions.

Figure 8-10: Comparison of axial power density
Figure 8-11: Comparison of radial power density

Figure 8-12: Comparison of axial thermal fluxes
The comparison of fluxes also shows a good agreement between DORT-TD/THERMIX and other codes. It is also observed that the diffusion solution agrees much better with the other diffusion counterparts, whereas the transport solution predicts a different value of the power and hence the fluxes. Since there is no reference solution for the benchmark, and DORT-TD/THERMIX is the only transport code participating in the benchmark, it is still difficult at this stage to determine whether the transport solution better represents the results. A closer look at the two-dimensional power maps reveals higher power peaks in the transport solution than in the diffusion solution. This may either be due to the deficiency in the way the total cross section was generated or due to the transport effects which were shown and discussed in Chapter 5 for stand-alone neutronics steady-state cases. Despite these small differences between transport and diffusion, the coupled code DORT-TD/THERMIX has shown to be predicting the core behaviour of the PBMR 400

![Graph of radial thermal fluxes](image)

Figure 8-13: Comparison of radial thermal fluxes

in much the same way as the other established codes.
Figure 8-14: Comparison of axial fast fluxes

Figure 8-15: Comparison of radial fast fluxes
8.5 Issues to consider in transient analysis

In the previous section, the steady-state problem (Exercise 3 was modeled with the newly developed coupled code. The results were also compared to those of other participants in the benchmark and good agreement was observed. In this section, a further verification effort is made, this time concentrating on transient analyses. The same PBMR400 OECD/NEA benchmark, wherein a number of transients postulated for the PBMR400 are described, is used. A selected number of these transients will be modeled with DORT-TD/THERMIX, paying attention to those that have a bearing to both neutronic dynamics and thermal-hydraulics. No comparison with other codes is done here because of the unavailability of such data at the present moment, therefore, only the diffusion and transport solution of the same code will be compared against each other with the idea of discerning with any differences that may arise due to transport effects in the transients.

Before starting with the transient analysis, it is important to discuss some issues related to the pebble temperature modeling, thermal conductivity, decay heat and xenon modeling as implemented and used in DORT-TD/THERMIX as these have shown to have a bearing on the overall behaviour of transients in the PBMR400.

8.5.1 Temperature distribution in the fuel pebble

The THERMIX-DIREKT code provides for two methods to calculate temperature of the fuel, namely, the so-called homogeneous model and the shell-model. In the homogeneous model, it is assumed that there is a uniform distribution of temperature
across the fuel pebble, and therefore the fuel and moderator are essentially the same, with the exception that for the moderator, only the temperature of the outer graphite of the pebble is considered. On the other hand, the shell model divides the fuel pebble into five shells and the temperature of the inner most shell is regarded as the maximum fuel temperature, whilst the average over the four inner shells is regarded as the fuel temperature. The moderator temperature is then computed to be the average of all five shells. The first model is obviously fraught with very extreme assumptions and can only be used for overly simplified calculations. For a reactor operating at a significant level of power, the assumption of uniform temperature is not valid because the central (fuel) region of the pebble will experience a higher temperature than the surface. The two most important consequences will be that (a) the maximum fuel temperature will be underestimated, thus resulting in the neutronics calculating higher powers and (b) the temperature at which the cross sections are tabulated i.e. the feedback temperature will in fact be wrong.

To illustrate this point by investigating the degree to which uniform temperature profile deviates from the actual temperature profile in a power generating pebble, the following parameters are defined:

\[ r \]: radial coordinate in the pebble geometry (cm)

\[ R_i \]: radius of the fuel zone of the pebble (2.5 cm)

\[ R_o \]: radius of the pebble (3.0 cm)

\[ T_{FZ}(r) \]: Temperature of the fuel zone \((0<r<R_i)\) (K)

\[ T_{Sh}(r) \]: Temperature of the pebble shell \((R_i<r<R_o)\) (K)
\[ T_o \quad : \quad \text{Temperature at the surface of the pebble} \quad \text{(K)} \]
\[ T_c \quad : \quad \text{Temperature at the centre of the pebble} \quad \text{(K)} \]
\[ P \quad : \quad \text{Power generated by pebble} \quad \text{(W/pebble)} \]
\[ \lambda \quad : \quad \text{Heat conductivity coefficient for graphite} \quad \text{(W cm}^{-1}\text{ K}^{-1}) \]

The above can then be used in steady-state heat equations (in radial coordinates) to derive the boundary conditions for the fuel zone and pebble shell as used in Kugeler and Schulten [44] as follows:

\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \lambda \frac{dT_{FZ}}{dr} \right) = -\frac{P}{4\pi R_i^3} \tag{8.1}
\]

\[
\frac{1}{r^2} \frac{d}{dr} \left( r^2 \lambda \frac{dT_{Sh}}{dr} \right) = 0 \tag{8.2}
\]

with the boundary conditions

\[ r=0 \quad : \quad \left( \frac{dT_{FZ}}{dr} \right) = 0 \]

\[ r=R_i \quad : \quad \left( \frac{dT_{FZ}}{dr} \right) = \frac{dT_{Sh}}{dr} \text{ and } T_{FZ} = T_{Sh} \]

\[ r=R_o \quad : \quad T_{Sh} = T_o \]

The temperature \( T_o \) at the boundary of the pebble is determined by the temperature of the coolant and the heat transfer coefficient as
\[ T_o = T_g + \left( \frac{P}{\alpha 4\pi R_o^2} \right) \]

where \( \alpha \) (in \( W \text{ cm}^{-2} \text{ K}^{-1} \)) is the heat transfer coefficient and \( T_g \) is the coolant temperature. In Equations 8-1 and 8-2 above it is assumed that the power density (i.e. \( \frac{P}{\frac{4}{3}\pi R_i^3} \)) is homogeneous over the fuel zone of the pebble.

Furthermore, the heat conductivity coefficient (\( \lambda \)) is assumed to be constant and equal for fuel zone and pebble shell. Solving the differential equations with the boundary conditions results in:

\[
T_{FZ}(r) = T_o + \frac{P}{4\pi \lambda} \left\{ \frac{3}{2R_i} - \frac{r^2}{2R_i} \right\} \quad 8.3
\]

\[
T_{Sh}(r) = T_o + \frac{P}{4\pi \lambda} \left\{ -\frac{1}{R_o} + \frac{1}{r} \right\} \quad 8.4
\]

This shows that the temperature is decreasing from the centre to the surface of the pebble. The maximum temperature at \( r = 0 \) becomes \( T_o + \frac{P}{4\pi \lambda} \left\{ -\frac{1}{R_o} + \frac{3}{2R_i} \right\} \). The maximum temperature differences of the fuel zone, pebble shell and the entire pebble becomes:

\[
\Delta T_{FZ} = \frac{P}{4\pi \lambda} \left\{ \frac{1}{2R_i} \right\} \quad 8.5
\]
\[ \Delta T_{Sh} = \frac{P}{4\pi\lambda} \left( \frac{1}{R_o} + \frac{1}{R_i} \right) \quad 8.6 \]

\[ \Delta T = \Delta T_{Sh} + \Delta T_{FZ} = \frac{P}{4\pi\lambda} \left( - \frac{1}{R_o} + \frac{3}{2R_i} \right) \quad 8.7 \]

For a pebble-bed with a power density of 10W/cm³ and a packing fraction of 61%, the power per pebble is 185W. If a heat conductivity coefficient of 0.2W/cm/K is assumed, the maximum temperature difference over the pebble becomes about 5°C. Obviously then, the homogeneous model for calculating the fuel temperature is inaccurate and therefore not used in this work.

Without going through the intimate mathematical derivations, it can also be shown that the shell model as currently used in THERMIX-DIREKT uses the following equations for temperature calculations:

\[ T_{FZ}^{ave} = \frac{1}{\pi} \int_{R_i}^{R_o} \frac{T_{FZ}(r)4\pi r^2 dr}{4\pi r^2 dr} = T_0 + \frac{P}{4\pi\lambda} \left\{ - \frac{1}{R_o} + \frac{6}{5R_i} \right\} \quad 8.8 \]

\[ T_{Sh}^{ave} = \frac{1}{\pi} \int_{R_i}^{R_o} \frac{T_{Sh}(r)4\pi r^2 dr}{4\pi r^2 dr} = T_0 + \frac{P}{4\pi\lambda} \left\{ - \frac{1}{R_o} + \frac{3}{2R^2} - \frac{R_i^2}{R_o^2} \right\} \quad 8.9 \]
The graphite temperature, averaged over the entire pebble, is equal to the volume weighted average of the average temperatures of the fuel zone and the pebble shell, and hence becomes

\[ T_{\text{ave}}^{\text{Peb}} = \frac{R_i^3 T_{\text{ave}}^{\text{FZ}} + (R_o^3 - R_i^3) T_{\text{ave}}^{\text{Sh}}}{R_o^3} \]

8.10

The above assumes that there is no temperature difference between a fuel kernel and the ambient graphite (i.e neglecting the coatings), which means that the average fuel temperature will be identical to the average graphite temperature in the fuel zones. This is a valid assumption if the thermal conductivity of the kernel is very large and the surface-to-volume ratio of the kernel is very small. Consequently, the difference between the average fuel temperature and the average graphite temperature becomes:

\[
T_{\text{ave}}^{\text{fuel}} - T_{\text{ave}}^{\text{Peb}} \approx T_{\text{ave}}^{\text{FZ}} - T_{\text{ave}}^{\text{Peb}} = \frac{R_o^3 - R_i^3}{R_o^3} \left( T_{\text{ave}}^{\text{FZ}} - T_{\text{ave}}^{\text{Sh}} \right) \\
= \frac{R_o^3 - R_i^3}{R_o^3} \left\{ \frac{6}{5R_i} \left( \frac{3R_o^2}{2} - R_i^2 \right) \right\} \frac{P}{4\pi\lambda} \\
= 3.935 \times 10^{-3} \left( \frac{P}{\lambda} \right)
\]

8.11

This shows that the difference between average temperature of the fuel and that of the graphite is proportional to the power and inversely proportional to the heat conductivity of the graphite. This difference is independent of \( T_o \) and of the temperature of the gas (coolant) as well as the heat transfer coefficient of the gas. Studies have shown that this difference can be as small as 36°C at steady-state conditions. This temperature difference albeit smaller for steady state calculations suggests that there needs to be a correction introduced in order to accurately model the fuel kernel temperature for fast
reactivity insertion transients where this difference may be larger. This correction was implemented in DORT-TD/THERMIX via the following relationship for the fuel kernel and the ambient graphite temperature:

\[
T_{\text{ave}}^{f_k} = \frac{\int_{0}^{r_{f_k}} T_{f_k}(r) 4\pi r^2 dr}{4\pi \int_{0}^{r_{f_k}} r^2 dr} = T_{\text{Amb}} + \frac{P}{4\pi \lambda_{f_k} N_{\text{gr}}} \frac{1}{N_{\text{gr}}} \frac{1}{5r_{f_k}}
\]

Where \( N_{\text{gr}} \) is the number of grains per pebble and \( r_{f_k} \) is the radius of the fuel kernel. The difference between the average temperature of the fuel and the temperature of the ambient graphite is now equal to:

\[
\Delta T_{f_k}^{\text{ave}} = T_{f_k}^{\text{ave}} - T_{\text{Amb}} = \frac{2}{5} \Delta T_{f_k}
\]

Where

\[
\Delta T_{f_k} = \frac{P}{4\pi \lambda_{f_k} N_{\text{gr}}} \frac{1}{2r_{f_k}}
\]

The importance of this correction will be demonstrated by showing the difference between using the shell model and the now newly implemented kernel correction model for fast transients.

Finally, for cross section feedback purposes, the “formal, theoretically and physically correct” Doppler feedback temperature is calculated as the average over the inner four shells of the pebble plus the fuel kernel correction term in Equation 8-12. For purposes of parametric studies, DORT-TD/THERMIX now has two options for calculating the Doppler feedback, namely the one just mentioned above, and secondly,
the average over the four inner pebble shells only. The latter, albeit inaccurate, is only used for purposes of comparing the DORT-TD/THERMIX results with the results from other codes which may not have this correction implemented yet. It may also be used for slow transient, where it is expected to yield accurate results although there is no computational incentive for doing so. The maximum fuel temperature still remains to be the temperature derived from the inner-most pebble-shell and the diameter of this shell is chosen to correspond to the diameter of one fuel kernel. The moderator temperature is taken to be an average over all five shells.

8.5.2 Thermal Conductivity

The heat transport through the bed of pebbles takes place partly by thermal conduction through the pebbles and partly by thermal radiation from one pebble to the other. The thermal conductivity of reactor materials, by its very nature is influenced by its environmental conditions, i.e. it is a function of both the temperature at which the material is exposed and the radiation dose (neutron fluence) that the material receives. Figure 8-16 depicts the behaviour of thermal conductivity of graphite as a function of these parameters. It is evident that thermal conductivity decreases with temperature for unirradiated graphite. For the highly irradiated graphite, temperature has virtually no effect on the thermal conductivity. At a certain threshold temperature (approximately 2500°C), conductivity of both the irradiated and unirradiated graphite converge towards the same value. This behaviour has been reported before [8] and has been attributed to the process of annealing, which essentially repairs to a high extent the lattice defects due to irradiation.
Currently, there are two conductivity models used in high temperature reactor pebble-beds. The model of Zehner-Schlünder [41] accounts for the heat transport from one pebble to the other. It has been verified in experiments, and it is recommended for the pebble-bed at low and medium temperature levels. On the other hand, the Robold model [42] takes special care of the heat transport through the openings between the pebbles of the bed by radiation. It also derives the effective thermal conductivity $\lambda_{eff}(T,D)$ which is preferred at higher temperatures, i.e. for $T > 1400$ °C.

The effective thermal conductivity of the pebble-bed for both the models is illustrated in Figure 8-17. It is drawn for the highest and for the lowest neutron fluence corresponding to the function $\lambda_{eff}(T,D)$ of the matrix graphite given above [43].
In the current version of the THERMIX-DIREKT code, only the Zehner-Schlünder correlation is used of the pebble-bed conductivity. It is given as a function of temperature for both unirradiated and irradiated graphite as follows:

\[
\lambda_{\text{unirr}}(T) = 61.1502 - 5.0309 \times 10^{-2} T + 0.2516 \times 10^{-4} T^2 - 5.0 \times 10^{-9} T^3
\]

and

\[
\lambda_{\text{irr}}(T) = 7.6098 + 1.0917 \times 10^{-2} T - 0.0348 \times 10^{-4} T^2 + 8.0 \times 10^{-10} T^3
\]
It is customary to use the irradiated graphite for transient analyses in cases such as the Depressurized Loss of Forced Cooling (DLOFC) because this correlation represents a conservative version of the transient. Furthermore, in THERMIX-DIREKT, unless otherwise specified, the conductivity of the pebble-bed is by default treated in a similar fashion as the conductivity of the fuel pebble shells, i.e. if the Zehner-Schlünder correlation is specified for the pebble-bed and no specific correlation or value is given for the pebble shells, the code automatically assumes a pebble-bed conductivity correlation in the pebble shells too. This assumption is important to highlight here because a slight change in the treatment of thermal conductivity can result in a large effect on the fuel temperature and hence the power of the reactor during transients. Moreover, in the transients that are analyzed in this thesis (based on the PBMR400 OECD/NEA Benchmark), a constant value of conductivity for the pebble-shells is specified, and this necessitated a slight code change. The effect of using the constant value against using the “standard/default” THERMIX-DIREKT correlation of thermal conductivity will be investigated.

8.5.3 Decay Heat

When the reactor is scrammed, the power does not immediately drop to zero, but falls rapidly before following a negative period determined by the longest-lived delayed neutron group. After a reactor shut-down, substantial amounts of heat continue to be released through the radioactive decay of both the fission products and transuranics in the fuel. The amount of heat released depends on the fission product concentration and therefore, the operating history of the reactor. Rigorous computation of decay heat release
over time can be carried out by solving a series of coupled differential equations for hundreds of fission products and their daughter nuclides. This computation is simplified by fitting a measured decay heat curve to a series of decay heat groups, analogous to delayed neutron groups. This functionality did not exist in DORT-TD/THERMIX and had to be implemented. THERMIX-DIREKT has the capability of modeling decay heat only by reading a supplied decay heat curve as stated above, which ordinarily would have been calculated by other codes using a certain decay heat standard, e.g. the DIN standard [47]. A simplified analytical decay heat model as implemented in the PARCS code was implemented in DORT-TD/THERMIX via the following formulations:

The total volumetric heat density, $q_T(r,t)$ with decay heat contributions is given by:

\[
q_T(r,t) = (1 - \alpha_T) \sum_{g=1}^{G} \kappa_g \sum_{g} \phi_g(r,t) + \sum_{i=1}^{I} \zeta_i D_i(r,t)
\]

where: $D_i(r,t)$ = Concentration of decay heat precursors in decay heat group I \([\text{J/cm}^3]\)

$\zeta_i$ = decay constant of decay heat group I \([\text{sec}^{-1}]\)

$\alpha_T = \sum_{i=1}^{I} \alpha_i = \text{total fraction of the fission energy appearing as decay heat, where I is the total number of decay heat groups}$

$\alpha_i$ = fraction of total fission energy appearing as the decay heat for decay heat group i

The decay heat precursors $D_i(r,t)$ can be represented by the following differential equation:

\[
\frac{\partial}{\partial t} D_i(r,t) = \alpha_i \sum_{g=1}^{G} \kappa_g \sum_{g} \phi_g(r,t) - \zeta_i D_i(r,t)
\]
An expression for the decay heat precursor concentration can be developed by integrating Equation 8-17 over the time interval $\Delta t = t_{n+1} - t_n$. This results in the following equation:

$$D_i(r, t_{n+1}) = D_i(r, t_n) e^{-\zeta \Delta t} + \alpha_i \int_{t_n}^{t_{n+1}} \left\{ \sum_{g=1}^{G} \kappa_g \sum_{f_e} (r, t') \phi_g(r, t') e^{- \zeta (t_{n+1} - t_n)} \right\} dt' \quad (8.18)$$

To solve the integral in Equation 8-18, a functional form for the time-dependent fission source density must be developed. Assuming the fission source density is constant at the past time step value over the time interval $t' \subset [t_n, t_{n+1}]$, the fission source density becomes:

$$\sum_{g=1}^{G} \kappa_g \sum_{f_e} (r, t') \phi_g(r, t') = \sum_{g=1}^{G} \kappa_g \sum_{f_e} (r, t_n) \phi_g(r, t_n) \quad (8.19)$$

Incorporating this approximation into Equation 8-18 and simplifying the equation gives the desired expression:

$$D_i(r, t_{n+1}) = D_i(r, t_n) e^{-\zeta \Delta t} + \alpha_i \left[ 1 - e^{-\zeta \Delta t} \sum_{g=1}^{G} \kappa_g \sum_{f_e} (r, t_n) \phi_g(r, t_n) \right] \quad (8.20)$$

It is assumed that in the steady-state conditions, the longest-lived decay heat precursor group is in equilibrium. The steady-state concentration is calculated by setting the time-dependent derivative in Equation 8-17 to zero and solving for the precursor concentration:

$$D_i = \frac{\alpha_i}{\zeta_i} \sum_{g=1}^{G} \kappa_g \sum_{f_e} \phi_g \quad (8.21)$$
Equation 8-21 is thus used to determine the initial conditions required for the transient solution of the decay heat.

### 8.5.4 Xenon Treatment

In order to treat the global and local power shifts resulting from xenon imbalances during power maneuvering in case of load-follow, it is necessary to keep track of the concentrations of these fission product and its global/local reactivity effects. For this reason, the treatment of xenon has been implemented in DORT-TD/THERMIX and is described for both equilibrium and transient cases. The time-dependent depletion of the fission product iodine and xenon which is used for updating the number densities and thus the absorption cross sections is described by the following differential equations:

\[
\frac{d}{dt} N_{\text{Iodine}}^{I}(t) = \gamma_{\text{Iodine}}^{I} \sum_{g=1}^{G} \Sigma_{fg}^{I}(t) \phi_{g}^{I}(t) \quad 8.22
\]

\[
\frac{d}{dt} N_{Xe}^{I}(t) = \lambda_{Xe}^{I} N_{Xe}^{I}(t) + \gamma_{\text{Xe}}^{I} \sum_{g=1}^{G} \Sigma_{fg}^{I}(t) \phi_{g}^{I}(t) - \lambda_{Xe}^{I} N_{Xe}^{I}(t) - \sum_{g=1}^{G} \sigma_{Xe,ag}^{I}(t) \phi_{g}^{I}(t) N_{Xe}^{I}(t) \quad 8.23
\]

Where  
\( N_{Xe}^{I} \) = nuclei number density of isotope Xenon

\( N_{\text{Iodine}}^{I} \) = nuclei number density of isotope Iodine

\( \gamma_{\text{Iodine}}^{I} \) = Iodine yield

\( \sigma_{Xe,ag}^{I} \) = xenon microscopic absorption cross section for a given energy group g.

\( \lambda_{Xe}^{I} \) = xenon decay constant
These parameters are all used in the code to calculate and update the concentration of xenon and iodine for each region/node at each time-step.

8.6 PBMR 400MW OECD/NEA Benchmark Transient Cases

Having discussed several issues which affect the transient behaviour in pebble-beds reactors, this section presents the results of transient calculations using the PBMR 400MW OECD/NEA benchmark test cases.

8.6.1 Cold Helium Ingress

This transient is an example of the importance of using the correct thermal conductivity and temperature treatment in a pebble. In this case, a bypass valve opening is simulated with the “cold” helium being injected into the core inlet plenum. A temperature ramp of 50 °C (i.e. 10% of nominal inlet temperature) is applied over 10 s, without changing any other reactor parameters such as mass flow, pressure or control rod positions. It is assumed that a reactor protection system would cause the valve to close again after 300 s, and the temperature would return to nominal value, again over 10 s. The transient history was followed for 600 seconds, and the fission power, maximum and average fuel temperatures were compared for both the transport and diffusion modes of the code. Sensitivity of the transient to different thermal conductivities is also illustrated by modeling the transient with the fixed conductivity value supplied with the benchmark specification, as well as using the standard THERMIX-DIREKT hard-coded thermal conductivity correlation.
It can be seen from Figure 8-18 that the reduction in the inlet temperature causes a steady but steep increase in fission power, reaching a maximum of about 115% of the nominal power due to increased moderation in the fuel. Upon returning the temperature back to the original value at about 300s, the power drops almost drastically and returns to about 102%. The results show that the transient is not very neutronically inclined since most of the initiating events are temperature driven and the neutronics only responds via the associated feedback effects, hence, there is a very small difference between transport and diffusion results in this case. However the results show a significant sensitivity of the transient to different thermal conductivities. Using a fixed conductivity as supplied with the benchmark specification yields almost 2% differences in the peak power as compared
to using the standard THERMIX-DIREKT conductivity correlation. It is important to note that the standard THERMIX-DIREKT thermal conductivity correlation is based on irradiated graphite data. Furthermore, it is important to realize that the difference in irradiated and unirradiated graphite can be large and it is of paramount importance that the correct thermal conductivity is used for this transient when safety analysis is performed. In case of doubt which conductivity to utilize, the irradiated thermal conductivity should be chosen for safety studies as this gives a conservative scenario as shown in the results above. This transient has very little effect in the fuel temperatures as shown in Figure 8-19 because the cooling effect is felt more on the pebble surface, and hence moderator temperature shows significant changes as shown in Figure 8-20.

Figure 8-19: Maximum and average fuel temperature during the Cold Helium Ingress
Figure 8-20: Moderator temperature changes during the Cold Helium Ingress

It can be concluded from Figure 8-20 that it is important to accurately model the temperature of the pebble so as to clearly and correctly distinguish the moderator temperature from the fuel temperature because the moderator temperature feedback effects are important for this type of transient.

**8.6.2 Depressurized Loss of Forced Cooling with and without Scram**

In modeling this transient, a depressurization is assumed to occur linearly over a period of 13s, with a resultant loss of forced cooling over the same period. Such a scheme could occur as a result of rapture (guillotine break) of the manifold connecting the power conversion system to the reactor unit. Helium will flow out of the containment into the
reactor building until the pressures are stabilized at 1 bar (from 90 bars). The eventuality of air entering the core and the subsequent oxidization of graphite is not taken into consideration in this case. The effects of natural convection should be included and since no scram assumed for the first case, re-criticality should occur. The transient is modeled with both the diffusion and transport modes of the code and is followed for 100 h. The analytical decay heat model which was implemented in the code is used as well as the decay heat curve supplied with the benchmark specification, and at given times, the fuel temperature, moderator temperature, fission power and decay heat power are reported. In the case where a scram is assumed, the same sequence of events is assumed i.e. a depressurization over a period of 13 s and at this time all control rods are inserted linearly over 3 s to scram the reactor. The effects of natural convection are included as before, but in this case, since a scram did take place, the reactor is expected to remain shut down, and therefore no re-criticality will occur.

![Figure 8-21: Fission and Decay Heat Power During a DLOFC with and without scram](image)

Figure 8-21: Fission and Decay Heat Power During a DLOFC with and without scram
For a depressurized loss of forced cooling (DLOFC), the prompt fission power will rapidly decrease and after a few minutes, become negligible compared to decay power as shown in Figure 8-21. Passive cooling processes will transport the decay heat from the core to the pressure vessel where it can be transferred to the environment by natural convection. This is obviously a slow process and will take days before equilibrium is reached. Due to the large thermal inertia in graphite, the temperatures increase very steadily and reach a maximum of about 1600 °C after almost one and a half days as shown in Figure 8-22.
It can be seen in Figure 8-21 that there is virtually no difference in transport and diffusion regarding the fission power and decay heat power. Furthermore, the analytical decay model implemented in DORT-TD/THERMIX agrees reasonably with the decay heat curve supplied with the benchmark specification, the small differences can be attributed to the simplified approach used in DORT-TD/THERMIX, where only $^{235}\text{U}$ fission products are assumed to produce heat but no Plutonium-like fission products are considered. Power drops rapidly to decay power in the case where there is scram induced, and drops slow for the case where there is no scram. The temperatures for the case where there is no scram are as expected slightly higher than those where there is scram because of the slow drop in fission power, so the reactor continues to produce fission power for a few more minutes when there is no scram without significant cooling, hence heating up the fuel. Finally, the maximum temperatures also show a slight difference between transport and diffusion, ~50°C and this is clearly a transport effect since the steady-state power is different for transport and diffusion hence there are some “hotter spots” in the core for transport than diffusion.

Although not shown in Figure 8-21, following the transient up to 100 h does not result into any recriticality occurring as expected. Two effects are supposed to bring the reactor back to criticality: firstly, the gradual decrease in decay power results in a cooler reactor, thereby increasing reactivity, and secondly, the xenon concentration decreases which also introduce a positive reactivity. However, re-criticality did not occur up to $t=100$ hours. This is a result of simplifying the design i.e. excluding bypass flow, assuming that heat is only deposited locally and also using a constant thermal conductivity value instead of using the established and more realistic correlations. It is
expected that for the actual design (without simplifications) recriticality would occur between 80-90 hours, although DORT-TD cannot at this stage model recriticality due to the criticality tracer not yet implemented.

8.6.3 Fast Control Rod Ejection

The control rod ejection accident is an assumed failure of the control rod mechanism pressure housing, such that the reactor coolant system would eject the control rods and drive shaft to the fully withdrawn position. It is a postulated accident that is a deviation from normal operations of the plant with a probability to happen less than $10^{-2}$/year. The consequence of this accident is a rapid reactivity insertion together with a power burst and an adverse core power distribution. The transient is terminated by Doppler reactivity effect of the increased fuel temperature, by the negative moderator temperature and eventually by a reactor scram caused by high neutron flux signal. In the PBMR400 benchmark, the sequence of events leading to a fast control rod ejection accident is such that the ejection of all 24 controls rods over 0.1 second duration is assumed. Obviously this is a highly unlikely event and this case was specifically postulated to have an unrealistically large reactivity insertion over a very short space of time. The correct implementation of kinetics equations and parameters in the code is thus verified in this type of a transient. The transient is followed for 60 seconds and the fission power and maximum fuel temperature are parameters of concern in this transient. It is also in this type of a transient where the details of a thermal hydraulic model are of importance, in particular, the correct fuel temperature feedback implementation with regards to the pebble and kernel models.
Since both the pebble shell and kernel model for fuel temperatures are implemented in the code, the transient was simulated with both models, to determine its sensitivity to the “correct” fuel temperature feedback treatment. The results are shown below:

**Figure 8-23: Fission power during a control rod ejection transient**

**Figure 8-24: Maximum fuel temperature during a control rod ejection transient.**
It can be seen from both Figure 8-23 and 8-24 that there are big differences in the fission power and the maximum fuel temperature peak depending on which fuel temperature model is used. When the shell model is used, (i.e. treating the temperature of the inner shell of the pebble as the fuel without taking into consideration that the kernels are embedded into a matrix of graphite) this results in very high maximum fuel temperature because the Doppler feedback to turn back the power is delayed due to the lowered thermal conductivity of uranium dioxide and the coatings which makes heat transfer even slower in kernel, thereby causing the fission power to surge by a factor of 120 before returning promptly to about 600% within 5 seconds. On the other hand, using the model that corrects the shell model to take care of fuel kernels explicitly results in a much reduced power peak and hence a much lower maximum fuel temperature peak. It is thus very important to use the correct fuel temperature treatment for this transient, especially for safety analysis purposes. The eventuality of how much fuel is damaged due to this very sharp power peak is not being dealt with here as this is not intended to be a safety study.

The results shown above are from the diffusion option of DORT-TD/THERMIX with full buckling treatment. The effect of using transport theory instead of diffusion, or using the buckling feedback or not, is illustrated in Figure 8-25. It can be seen from this figure that other than slight power shift in the peak, diffusion and transport theory yield almost the same power peak result for this transient. Ignoring the buckling feedback results in the under-estimation of the fission power peak because of the inaccurate treatment of the leakage.
In the cross section libraries, neutron velocities were supplied for each material and each spatial region in the reactor core. A parameter study was performed for this transient in particular to discern with the importance of treating neutron velocities explicitly for each zone as against using core averaged neutron velocities. The importance of this is that it would reduce the amount of data to be interpolated in the cross section tables and hence increase the efficiency of the calculation whilst accuracy is preserved. As shown in Figure 8-26, there is a marginal decrease in the fission power peak when core averaged neutron velocities are used as opposed to using spatially
resolved neutron velocities. Using a constant kappa value, i.e. constant energy release for all materials or changing the kappa value for different materials has hardly any effects on the results.

In order to compare the differences between transport and diffusion on a spatial grid i.e. to compare local deviations, snapshots of the power distribution during different stages of the transient were taken. The stages of interest compared are at time $t = 0.1 \, \text{s}$ which is at the onset of the transient, then at $t = 0.2 \, \text{s}$, and then at the power peak and 2 seconds after the power peak. It is important to note that the power peak is reached at different times for transport and diffusion due to different rod worths for both, and hence different reactivity insertion. As it can be seen in Figure 8.27 through Figure 8.30, the differences between diffusion and transport is consistent, becoming larger at the power peak, and

![Power for spatial/group-wise neutron velocities](image-url)
then diminishing towards the end of the transient. The power is rapidly shifting towards the top of the core as the power shape deteriorates due to the ejection of the rods.

Figure 8-27: Axial power distribution at t = 0.1 sec during a CRE transient

Figure 8-28: Axial power distribution at t = 0.2 sec during a CRE transient
Figure 8-29: Axial power distribution at the power peak during a CRE transient

Figure 8-30: Axial power distribution 2-sec after the power peak during a CRE transient
Finally, to confirm that there wouldn’t be any effect on the transient results due to using a higher quadrature order in the transport calculations, a calculation was performed using the $S_8$ quadrature and as shown in Figure 8-31 below, this does not affect the results at all. It must once again be recalled that the cross sections used in these cases are only based on $P_0$ scattering and also, DORT-TD cannot utilize the beta values in the library, instead we utilize effective betas (valid for the whole core) and these are generated from direct-adjoint weighting of material-wise betas in steady-state. These deviations from the actual benchmark library may also have an effect on the results.

Figure 8-31: CRE – lower v/s higher quadrature
8.6.4 Slow Control Rod Withdrawal

This is another reactivity insertion transient although much slower than the CRE case. In this case, a complete withdrawal (250 cm to 50 cm) of all control rods from 0 to 200 s (i.e. speed of 1 cm/s) is postulated. The transient is followed for 600s and the fission power and maximum fuel temperature are required output. The transient was modeled using transport and diffusion theory, the fixed benchmark conductivity and the standard THERMIX conductivity correlations. Once again, the inserted reactivity during the rod withdrawal amounts to 1466 pcm for both transport and diffusion calculations as was the case with the fast control rod ejection case. The results are shown below:

Figure 8-32: Fission power during a slow control rod withdrawal
Unlike in the rapid control rod ejection case, the slow control rod withdrawal results in a sharp but somewhat gradual increase in fission power and reaching a maximum of about 210% of the nominal power. There is a small difference between transport and diffusion results in this case as was the case with the CRE. It must be mentioned here that the different shapes in diffusion and transport results stems from different control rod worths curves for diffusion and transport. Since the overall reactivity is the same, both transient solutions assume the same peak value, 210% of the nominal power. The transient is however sensitive to thermal conductivity value used and as seen above, the standard THERMIX thermal conductivity correlation yields higher fission power whilst the fixed conductivity value is much conservative. The control rod cusping effects are evidence of the “primitive” control rod movement model implemented in DORT-TD, which simply takes into account volumetric material mixing only during the control rod movement. A better model would eliminate the unphysical behaviour in the fission power.

Finally, another major difference between this transient and the fast control rod ejection transient is the fact that due to the smaller and gradual reactivity insertion, the fuel temperature increases very slowly and reach a maximum of about 1450°C when the fixed conductivity value is used and much less (about 1300°C) when the THERMIX standard conductivity correlation is used, as shown in Figure 8-33.
The importance of using the correct thermal conductivity is also demonstrated in this transient by the 150°C difference in maximum fuel temperature between two thermal conductivity models used.

8.6.5 100-40-100% Load Follow

Responding to a change in power demand, so-called load following can be achieved in the PBMR by changing the helium inventory in the system. The amount of heat produced by the reactor is approximately linear with the helium mass flow rate through the core. If the power demand drops, the control system can reduce the mass flow rate and effectively reduce the cooling capacity of the flow. In the PBMR400, the
load follow designed for is the load change from 100% to 40% and back to 100% of the nominal power. Simulating this transient is necessary to test the correct implementation of xenon equations as this type of a transient may initiate xenon-induced spatial power oscillations. In order to model such effects, a reduction in reactor inlet coolant mass flow from nominal (192.7 kg/s) to 77 kg/s (40% of nominal) from t = 0s over 8 seconds is assumed. The mass flow ramp is assumed linear. The reactor outlet pressure is decreased over the same time from nominal (90 bar) to 40% and this results in a reduction in reactor power level from nominal 400 MW (100%) to 160 MW (40%) from t=0 over 8 seconds. This power ramp is also assumed linear. For three hours thereafter (8s – 10800s), no change in input parameters is made. Later, from 10800s – 10808s, an increase in reactor inlet coolant mass flow from 77 kg/s (40% of nominal) back to 192.7 kg/s is assumed. The reactor outlet pressure is increased linearly back to nominal at the same time, resulting in an increase in reactor power level from 160 MW to 400 MW, again over 8 seconds. The reactor total power is thus a fixed target condition. The total power and average and maximum xenon concentration are required output parameters for this transient and they are shown in Figure 8-34. Only the diffusion results are shown for this transient due to the enormous amount of computational time and very slow convergence of the code because of the continuous control rod movement in this case to compensate for the negative reactivity that results from dropping the power to 40% and also for the positive reactivity that results from increasing the power back to 100%.
From Figure 8-34, it can be seen that reducing the mass flow and the pressure will result in the reactor core warming up as it cannot transfer all its heat to the gas, and will lessen the power production as can be expected from the negative temperature coefficient of reactivity for the core. Initially, the xenon concentration will buildup and will continue to do so to the extent that the power cannot stay at 40% if the control rod is not moved to compensate for this negative reactivity. As shown in the figure, the power dips slightly lower 40% initially and the control rod is adjusted to keep the power at 40%. After three hours when the power is brought back to 100%, the xenon concentration decreases steadily to almost its initial value as xenon is consumed. The results are consistent with known physics and thereby confirming the correct implementation of the xenon dynamics in DORT-TD/THERMIX.
8.7 The effect of using higher order transport theory for PBMR transients

In the previous sections the DORT-TD/THERMIX code was used to model PBMR400 transients as prescribed in the OECD/NEA benchmark. It was explained that the benchmark exercise provided a two-group cross section library based on what is readily usable by diffusion theory based codes. For transport theory codes, the scattering matrices were supplied as $P_0$ and a $P_1$ transport correction was applied to the total cross section and then the self-scatter cross section is calculated in a traditional way i.e. (selfscatter = total - absorption – outscatter). The results presented thus far have shown a small difference between diffusion theory and transport theory but nonetheless the steady-state power shapes have shown some differences and therefore these differences appear in the transients too. Although the peak powers are the same for example in the slow CRW case, the transient trends are significantly different, e.g. different points in time where the maximum power is attained, different slopes at different times etc. The thermal-hydraulics feedback effect seems to be very similar for diffusion and transport, since the core responds very similarly with both cases. However, the transport correction simply implies that problems with linearly anisotropic scattering can be replaced by problems with isotropic scattering, provided that the scattering cross section (and the total cross section) is reduced by the amount $\mu_s\Sigma_s$ [45]. It is therefore important to understand transport correction as exactly what it is: an approximation of some sort, because the only situation where the transport correction is exact is when mono-energetic neutrons are considered, which not the case for reactor problems is. The two-group cross sections provided with the benchmark specification to a larger extent still assume linearly
isotropic scattering. This may be the reason why small differences between transport and diffusion were observed for the PBMR 400 transient calculations.

In order to clarify this issue, higher order transport ($P_1$ and $P_3$) six group cross sections were generated using the MICROX 2 code. In this way, a larger number of groups, higher scattering order as well as higher quadrature could be used to finally confirm if there are really small differences between transport and diffusion calculations for PBMR analysis. The PBMR 268 model discussed in Chapter 5 was used for this purpose. Cross section tables were generated with three state parameters i.e. four fuel temperatures (300K, 800K, 1400K, 2400K), six moderator temperatures (300K, 800K, 1100K, 1400K, 1800K, 2400K) and three xenon number densities included for the fuel materials, while for all the non-fuel materials no fuel temperature or xenon variations are included. The buckling dependency of the cross sections was eliminated in this case for simplicity purposes.

It is important at this stage to mention a few differences between the PBMR400 and the PBMR268 designs so that the reader is not confused when interpreting the results. The PBMR268 design has an annular core in the same way as the PBMR400 design except that the central graphite region in the core of the PBMR268 design is a dynamic column made up of graphite spheres with the same size as the fuel spheres, whereas in the PBMR400, the central graphite column is fixed solid graphite. Needless to mention that the power is 400MWth and 268MWth in both designs respectively. Finally, the PBMR400 design has a shut down rod channel in the centre of the core and this is not the case for the PBMR268. The reserve shut down system for the PBMR268 is located in the side reflector where the control rods reside. A model for this design was developed in
DORT-TD/THERMIX and steady-state and transient calculations were performed. The steady-state results are shown below:

![Keff PBMR 268 six group data](image)

**Figure 8-35: K\text{eff} comparison for the PBMR 268 six group models**

Figure 8-35 shows a comparison of \(K_{\text{eff}}\) when using diffusion and higher order transport models. It can be seen that there are slight differences between diffusion, \(P_1S_2\) and \(P_1S_4\), but almost no differences any more for \(P_1S_8\) and \(P_3S_8\). This is a consistent result because with an increasing accuracy, and asymptotic behaviour is observed, however, the difference between transport and diffusion in general is very small. The same behaviour can be seen in the comparison of power distribution, where only \(P_1S_2\) seems to be slightly larger peak powers than the rest but this behaviour is hardly physical because it is well known than for lower quadrature the accuracy of transport calculations is sometimes
compromised, hence the visible differences between \( P_1S_2 \) and \( P_1S_4 \), and small differences \( P_1S_8 \) and \( P_3S_8 \).

![Axial Power Density Distribution PBMR268 six group data](image)

**Figure 8-36: Axial Power Density Distribution Comparison**

The effect of the void region can clearly be seen in the above figure where diffusion slightly deviates from the other transport solutions at the top of the core around the void region for diffusion.

The coupled steady-state results show a good agreement between the diffusion and transport solutions except for very small deviations in both the eigenvalue and the power density. The next step is to confirm if the same behaviour is observed for transients. Three representative transients were chosen for this illustration, namely: a fast reactivity insertion transient (control rod ejection) and two slower transients (the control rod withdrawal and the cold helium ingress. The sequence of events for each transient is the
same as was described for the PBMR400 cases and therefore will not be repeated; only the results are shown.

![Control Rod Ejection Transient - PBMR268 six group data](image)

**Figure 8-37: Control Rod Ejection Transient Comparison of different models**

The control rod ejection transient was simulated with a reactivity insertion of 1587 pcm for all cases and the standard THERMIX shell model was used as temperature feedback. Figure 8-37 above shows the relative power for the first 1.0 seconds and it can be seen that P1S4, P1S8, and P3S8 lie on top of each other hence only the P3S8 curve is visible here. There are visible deviations for P1S2 from higher quadrature orders and even higher deviations for diffusion. This is a consistent result because the better the transport solution is, the close the results move towards the “reference” solution (P3S8), and hence an asymptotic behaviour with model refinement. The same effect, or even stronger can be seen from the case of a slow control rod withdrawal shown in Figure 8.34, where the
transport solution predict much higher power peak during the transient. At the end of the transient however, both the transport and diffusion solution stabilizes at exactly the same value of about 125% of the power.

Figure 8-38: Slow Control Rod Withdrawal transient comparison for the PBMR 268
Finally, a slower transient, the cold helium ingress, further shows no differences at all between diffusion and transport as shown in Figure 8-39. This further illustrates the fact that most of the transport effects seen here come from different control rod worths while the thermal-hydraulics response of the core is very similar as seen in the cold helium ingress transient shown above.

8.8 Time-step control and sensitivity studies

One of the capabilities of the coupled code is the ability for the neutronics module DORT-TD to self-regulate the time-step size proposed by the thermal hydraulics module. As discussed earlier in Chapter 7 in a given transient calculation, THERMIX-DIREKT sets the initial time-step size and the neutronics module evaluates this time-step size for its suitability by comparing it with the truncation error of a simple exponential. If this
proposed time-step size is larger for DORT-TD, it is then subdivided into several smaller
time-step sizes and data is then exchanged between the first and last time-points. This is
illustrated in Figure 8-40 for the control rod ejection transient in the PBMR 400MW.

Figure 8-40: Time-step adjustment in DORT-TD during a Control Rod Ejection

In the above diagram, THERMIX sets an initial time-step size of 10 ms. DORT-TD starts off with very small time-step sizes of less that 2 ms and then increases these accordingly until it reaches the proposed 10 ms time-step size. At problem time 0.1 s, when the transient starts i.e. when the control rods are ejected, the code proceeds with the time-step size of 10 ms but almost instantly, due to sharp reactivity changes, the time-step size is reduced significantly until it reaches below 1 ms. As the power peak is reached at around 0.7 s problem time, the time-step size is back at 10 ms because there is no reactivity changes at this point, and almost immediately, when the power begins to come
drop due to Doppler feedback, the time-step size is reduced to smaller time-steps again. At the end of the transient when the power is back at 100% at problem time 1.4 s, the time-step size is back at 10 ms again because the reactivity is almost constant from this point onwards.

This capability has proven to be very effective in accelerating the computational time, yielding typical run times of approximately 1 hour for the control rod ejection transient in diffusion mode, using the 2.2 GHz Pentium 4 PC for 1 ms time step size on a mesh of 30000 nodes (250 axial and 120 radial). The run time is divided almost equally between neutronics and thermal hydraulics. For the same transient running $S_4$ transport, two energy groups, the CPU time is 3.5 hours where 15% of the time is spent on THERMIX and 85% of the time is spent on DORT-TD. These are quite reasonable run times especially for transport calculations which can take much longer in other codes. The timestep size can still be increased based on the nature of the transient and lesser CPU times can be achieved.

In order to evaluate the sensitivity due to time-step size, calculations were performed for a fast reactivity insertion transient and a slow transient varying the time-step size arbitrarily. As a representative fast transient, the control rod ejection was once again chosen as a case in point, whilst the cold helium ingress transient was used as a representative slow transient in the PBMR 400 benchmark. The results of sensitivity studies for both cases are shown in Figures 8-41 and 8-42. As observed in Figure 8-41, for a slow transient like the cold helium ingress transient, there is a possibility of using time-step sizes of up to 2s seconds without loosing the accuracy. It can be seen that going to time-step sizes as big as 5s begins to deteriorate the accuracy of the calculation.
Figure 8-41: Time-step sensitivity in a slow transient

Figure 8-42: Time-step sensitivity in a fast control rod ejection transient
On the other hand, when considering a fast reactivity insertion transient, the choice of time-step size is very stringent. Using time-step sizes of more than 20 ms result in unphysical results and this can be clearly seen in Figure 8-42, where 30 ms shows an unphysical shifting of the power and any larger time-steps thereafter (50 ms and 100 ms) shows a very distorted power shape with unphysical cusps at the power peak.

8.9 Summary

This chapter presented two main activities, namely, verification and validation of the coupled code DORT-TD/THERMIX and investigation of the benefits of using higher order transport models in PBMR transient analyses. For the first part, the PBMR400 OECD/NEA benchmark was used as a basis. Two group nuclear cross sections supplied with the benchmark specification were utilized. These were generated for diffusion codes and therefore the scattering matrices supplied were $P_0$ and the total cross section corrected to $P_1$. Firstly the steady-state coupled exercise was simulated with DORT-TD/THERMIX using both the diffusion and transport mode of the code, and the results were compared with those of other participants. A very good agreement was observed between the codes and the DORT-TD/THERMIX diffusion option. There were small but visible differences between DORT-TD/THERMIX transport when compared to diffusion theory based codes, evidence of some transport effects. However the overall observation for this part was that the differences are quite small.

Several transients were also selected from the benchmark specification and were simulated with both diffusion and transport options of the coupled code. There were no comparisons done with other participants because no results were submitted yet.
Different parametric studies were carried out to determine the sensitivity of the transients to certain input parameters. It was observed in general from the results that for slow transients like the Depressurized Loss of Forced Cooling and the Pressurized Loss of Forced Cooling, a simple model for temperature feedback, the shell model, would suffice to accurately model these transients. It is however important to carefully select the correct thermal conductivity model or correlation for these transients because they are mostly temperature driven and therefore very sensitive to thermal conductivity. Moreover for safety analysis purposes it is also important to carefully choose which graphite data to use i.e. irradiated or unirradiated graphite as this can result in significant differences in transient results.

On the other hand, fast transients, in particular, the control rod ejection case, exhibit small but significant differences between transport and diffusion, but most importantly, they are very sensitive to how the fuel temperature feedback is modeled. The simple shell model has shown to under-predict the Doppler temperature feedback and result in very higher power peaks. When the correct fuel temperature feedback model is implemented by correcting the shell model with a factor to explicitly take the fuel kernels into account, the power peak is significantly reduced. These types of transients are also sensitive to thermal conductivity model in the same way as the DLOFC has shown to be.

The overall observation other than the mentioned sensitivities is that with the provided benchmark cross sections, there is a reasonable agreement between the transport and diffusion.

In order to present a flawless comparison between transport and diffusion theory, i.e. without simplified transport cross sections as was the case with the PBMR 400
benchmark cross sections, a new set of cross sections was generated in six energy groups, and higher scattering moments, $P_1$ and $P_3$. The results of using this new cross section library have shown that for slow transients, there is no effect when using either diffusion or transport cross sections. There is however some visible transport effects in fast transients but there is no need for higher quadrature than $S_4$ and no need for scattering moments higher than $P_1$.

In comparing the PBMR400 two group cross section cases and the PBMR 268 six group cross section cases, it can be concluded that diffusion and transport agree better when a higher number of energy groups is used, more than the two groups used in the PBMR400 where larger differences we seen than in the multigroup case. It is therefore advisable to use more than two energy groups, but a low transport approximation or even diffusion maybe enough for transients. It can be stressed at this point that despite the outcomes of the study, there are several issues that speak for the usage of transport theory rather than diffusion, especially for safety analyses purpose:

(1) The power shape in steady-state and also during transients may be different between transport and diffusion, which may affect some safety-related quantities like maximum fuel temperatures.

(2) The modeling of the control rod is apparently problematic, since the description of the rod movement and also of the differential control rod worths are significantly different, which becomes particularly obvious in transients initiated by control rod movement.

(3) Transport theory gives the best estimate of core feedback effects, although the core responds very similarly to the thermal-hydraulic changes, whether using
diffusion and transport. However this may be slightly different if the power
distribution is shifted towards the top void, for example, when considering fresh
cores. Then the void region may become more significant and may have larger
effects.

In conclusion, all the above-mentioned activities have provided a thorough
benchmark exercise for the verification and validation of the DORT-TD/THERMIX
coupled code.
CHAPTER 9
CONCLUSIONS AND RECOMMENDATIONS FOR FUTURE WORK

9.1 Conclusions

This thesis presents the application of advanced deterministic neutron transport methods for the safety analysis of the pebble bed modular reactor. In order to perform the analysis, a code system has been developed that couples neutronics and thermal hydraulics with options of using both diffusion and transport theory. This coupling has been developed in order to come to a more detailed and realistic simulation of the reactor, rendering the assumptions superfluous that otherwise would have to be made concerning time evolution of the boundary conditions of the two systems. The ultimate objective of this work was to make a determination, based on detailed modeling and analysis, of whether diffusion theory is adequate for the safety analysis of this reactor type, given the known deficiencies of this theory when applied to certain features of this design. In order to arrive to this conclusion, models were developed and numerous studies were carried to validate and verify the models. From the results obtained, we believe that the studies carried out in this thesis make a unique contribution to contemporary knowledge of the subject, and these contributions are summarized as follows.
9.1.1 Two-Dimensional $S_N$ Transport Models

In order to make a case for the need of using advanced deterministic transport methods for both steady-state and transient analysis of high temperature reactors of pebble-bed type, a transport model of the PBMR 268MW core was developed using the DORT code. Parametric studies were carried out to optimize the model for both accuracy and efficiency. In the process, it was discovered that the reactor model was not highly impacted by the number of quadrature and scattering order as well as nodalization. It was however noted that the number of energy groups impacted the accuracy of the model. It was concluded that the PBMR 268MW core can be accurately represented with a model based on $P_1S_4$ and at least four energy groups in steady-state. This refined model was compared with nodal diffusion solution generated from the NEM code using the same set of cross sections. The NEM code applied in the standalone steady-state studies was not modified to treat the directional dependent diffusion coefficients in the void region at the top of the core in the PBMR. What was done simply was taking the graphite cross sections and diluting them by a factor of 1000 or so, thereby yielding small total and transport cross section and consequently a huge diffusion coefficient. In this way, it was been proved that when the diffusion code is used without directional dependent diffusion coefficients (i.e. a transport modification) the void region causes big differences between the transport and diffusion solution, thereby rendering the diffusion theory inaccurate. For an accurate high fidelity analysis, a transport model has to be used or otherwise modifications are necessary in the diffusion theory code to treat the void region in a transport sense through the use of directional dependent diffusion coefficients. It became
important to investigate how the differences discovered between transport and diffusion could affect the transients in the PBMR especially for safety analysis.

9.1.2 Three Dimensional $S_N$ Transport Models

Accurate modeling of transients and safety analysis requires proper treatment of control rods such that control rod worths are accurately predicted. Since the main tool being used in this study, the DORT code is limited to only two dimensional geometry, it was necessary to develop three dimensional models to verify the control rods worth calculated with DORT. This is particularly important because for two dimensional models, control rods in the PBMR are treated as a cylindrical grey curtain represented by a known Boron number density and this is done beforehand using the method of equivalent cross section (MECS) or even the equivalent boron concentration method (EBC). To evaluate the accuracy of using this scheme (grey curtain representation of control rods), a three dimensional model which treats all control rods in the PBMR explicitly, was developed using the TORT code. To further verify the developed model, a detailed MCNP model was also developed. From the control rod worths studies carried out and the associated comparisons between TORT, DORT and MCNP, it can be concluded that the grey curtain representation of the control rods in the PBMR is quite reasonable, provided that the control rods cross sections are accurately computed. This was sufficient information to move on to coupled calculations and transient analysis.
9.1.3 Coupling neutron transport to thermal hydraulics

Two existing codes, DORT-TD, a time-dependent $S_N$ neutron transport code with a diffusion option, and THERMIX-DIREKT, an HTR core thermal hydraulics code, were coupled to provide an integrated code system with multiple capabilities. The coupling process included the incorporation of a multi-dimensional cross section data routine and the associated interpolation routine to interpolate and update cross sections at every timestep. In order to cover all postulated transients in the PBMR, further important features were implemented in the code such as a detailed analytical decay heat model which is important for slow heat-up transients such as the depressurized loss of forced cooling (DLOFC), and the xenon dynamics model which is important for transients that would necessitate taking the xenon dynamics into account like the load follow transient. The xenon model is not only necessary for the xenon transients but also inevitable for the steady-state calculations i.e. getting the correct xenon number densities for cross section interpolation, for calculation of the macroscopic cross sections in the neutronics calculation etc. If this is not done correctly, one would never get the eigenvalue prediction correctly because xenon amounts to approximately 2500-3000 pcm of reactivity in the core (i.e xenon equilibrium v/s xenon-free core). Furthermore, an accurate fuel temperature feedback model which takes into account both the differences between fuel kernel temperature and the temperature of the ambient graphite was also implemented into the code. This proved to be very important for transients which result into fast reactivity insertion such as the control rod ejection. Finally, a buckling feedback model which is uniquely important for pebble-bed reactors to accurately model the
leakage was implemented for the diffusion track of the code and has also proven to have a significant effect on the transients. A partial implementation for the transport track also exists. In a nutshell, a coupled code system DORT-TD/THERMIX, with multiple capabilities to model both slow and fast transients was developed.

9.1.4 Verification and validation

The developed coupled code system was verified using the established PBMR 400MW benchmark with the provided two group cross section libraries, a given pebble thermal conductivity model and decay heat curve. One coupled steady-state exercise and six different transient exercises prescribed in the benchmark specification were simulated with the code. The objective of this step was two-pronged, namely: verify the code against other codes and also determine the adequacy of diffusion theory in modeling the PBMR transients when compared to the transport solution. A good agreement between DORT-TD/THERMIX and other codes from the benchmark was observed in the coupled steady-state exercise. In transient analysis, no data from other codes was available to compare with and only DORT-TD/THERMIX diffusion and transport tracks were compared against each other. Different parametric studies were carried out to determine the sensitivity of the transients to certain input parameters. It can be concluded from the results that that for slow heat-up transients, a simple model for temperature feedback, the shell model, would suffice. Furthermore, it can also be concluded that it is important to carefully select which graphite data to use i.e. irradiated or unirradiated graphite and hence select the correct thermal conductivity model or correlation for these transients.
because they are mostly temperature driven and therefore very sensitive to thermal conductivity.

For fast reactivity insertion transients, in particular, the control rod ejection case, small but significant differences between transport and diffusion were observed and also the fact that such transients are very sensitive to how the fuel temperature feedback is modeled. The simple shell model has shown to have the tendency to “delay” the Doppler temperature feedback and thereby resulting in very higher power peaks. When the “correct” fuel temperature feedback model is implemented by correcting the shell model with a factor to explicitly take the fuel kernels into account, the power peak is significantly reduced. These types of transients are also sensitive to thermal conductivity model in the same way as the DLOFC has shown to be. The overall conclusion other than the mentioned sensitivities is that with the provided two-group benchmark cross sections, there is a reasonable agreement between the transport and diffusion.

9.1.5 Effect of higher order transport methods on PBMR transients

Realizing that the cross sections provided in the PBMR400 benchmark were meant for diffusion codes and therefore adjusted for transport theory based codes, one can appreciate the fact that such data does not provide a firm basis for conclusions on whether the diffusion theory is adequate for PBMR safety analysis or not. In order to eliminate any uncertainty due to the approximations during the cross section generation process, a new set of cross sections utilizing higher scattering moments and a larger number of energy groups (six groups) was generated for the PBMR 268 design. Selected
transients were analyzed and from the results of using this new cross section library it can be concluded that for slow transients, there is very small effect when using either diffusion or transport cross sections. There is however some visible transport effects in fast transients but there is no need for higher quadrature than S₄ and no need for scattering moments higher than P₁.

In summary, this study was able to show that there are significant deviations between transport and diffusion for the steady-state which may have a potential influence in design and safety calculations for example higher power peaks at interfaces to reflectors, other control rod worths, different behaviour at transition to void regions etc. Although the integral parameters like reactor power are very similar, local quantities reveal a deeper insight on the deviations because for example temperatures are quite different between transport and diffusion as was shown in this study. The developed coupled code can clearly be used as a reference tool which is capable of performing parameter studies whose capabilities e.g. usage of higher scattering moments, quadrature sets, importance of directional dependent coefficients, usage of either spatially resolved or group-wise neutron velocities and kappa energy release values, importance of buckling feedback in the cross sections (turning the buckling feedback on and off) did not exist before.
9.2 Future Work

Although this study has achieved almost everything it sought to achieve, there are certain activities that could not be pursued because of time constraints which could add more value to the work performed in this study. These activities are listed and summarily discussed in the sections below.

9.2.1 Buckling feedback implementation in DORT-TD/THERMIX (transport)

In the current version of the code buckling feedback is only accounted for in diffusion mode and not in the transport track. This was the case because implementing the necessary code changes in DORT-TD for this purpose proved to be a formidable task, given the time available. On the other hand, the results have shown significant differences when the buckling feedback is modeled or not. In order to circumvent this task, an adhoc solution was to use the steady-state diffusion buckling in transport and fix it during the transient. In this way one does not expect this parameter to change significantly during transients. When comparing the results of fully implemented buckling feedback in diffusion and those of a fixed steady-state buckling, the differences were much smaller than the case where the buckling feedback is ignored completely. It is therefore planned that a variable buckling feedback model be implemented in the transport track of the code in the future.
9.2.2 Improvement of the model for control rod movement

The current control rod model utilized in DORT-TD/THERMIX is a simplified one in which material mixing is introduced within a mesh where the material change occurs. In this way, the mesh can be kept unchanged and only cross sections in that mesh are weighted with the relative volume fraction of Boron-10 and Carbon respectively. This model has proven to be problematic when a node is partially rodded, because there appears a so-called cusping effect if the control rod cross section is incorporated using the volume fraction only. This occurs inherently because there is a flux depression in the partially rodded region leading to a smaller rod worth. These cusping effects were observed to be somewhat pronounced in the case of a slow control rod withdrawal. There are different ways to address this problem and one of such improved model is the so-called “quasi-continuous” control rod movement, in which the control rod position is chosen and all surrounding meshes are adapted in size, so that no small meshes can occur. This method already exists in DORT-TD but it only allows moving the control rod within a region with a single material, so since there are multiple layers of material in the PBMR benchmark test cases, the existing model will need to be updated to make it more appropriate for this reactor type.

9.2.3 Implementation of a point kinetics model

Although full neutron kinetics is required for the accuracy of reactor calculation, some transients in the PBMR may well be handled using a simplified point kinetics model because of their nature. At some point during the transient like DLOFC without scram,
detailed neutronic calculations become almost meaningless because there is not much going on neutronically in the core after a few minutes after the depressurization, where all the power in the reactor has been reduced to decay heat. Continuing with full neutron kinetics calculations becomes an unnecessary time-consuming effort and use of a point kinetics model becomes attractive and can speed up the calculation by several orders of magnitude. This also applies to the load follow transient, which has shown to be very computationally involved. However, for the point kinetics model to work properly in the code, it is necessary to generate the appropriate kinetics parameters from steady-state calculations. This can already be done in DORT-TD, i.e. both prompt neutron lifetimes and effective delayed neutron fractions can be generated. The quasi-core averaged beta effective values are produced from the material-wise betas (i.e. those supplied with the cross section library) by direct/adjoint weighting, and then these effective values are used in the transient diffusion/transport calculations. These effective betas can also be correct values to use in point kinetics calculations because point kinetic calculations do not utilize the spatially varying betas anyway, and therefore DORT-TD offers an opportunity to provide very accurate transport-based values for kinetic parameters, a feature that is absent in many codes. The only deficiency of the code in this regard currently is the fact that spatially resolved betas cannot be used in transient mode directly; instead, only pre-generated effective core-averaged values can be utilized as explained above. This modification is envisaged to be implemented in the future.
BIBLIOGRAPHY


9. Knufer H., “Preliminary operating experiences with the AVR at an average hot gas temperature of 950 °C” Nucl. Eng & Design 34 (1975)


12. PBMR Basic Core Design Report, document number 002979-34/1A


20. Argonne Code Centre: Benchmark Problem Book”ANL-7416, Suppl.2, Argonne National Laboratory, USA


42. Heat transport and afterheat removal for gas cooled reactors under accident conditions, IAEA-TECDOC-1163 (January 2001)

43. Data and Boundary Conditions to be used in VSOP and TINTE PBMR 400MWth reactor models. PBMR Internal Report, Report number: 022028, (June 2004)

44. Kugeler, K and Schulten, R., Hochtemperatur-reaktortenchnik, Springer-Verlag, 1989

Appendix A

EXAMPLE OF DORT-TD INPUT FILE (LOAD FOLLOW TRANSIENT)

BLOCK1
@
@ Transport
  Theory=0

@ Adjoint calculation
  Adjoint=0

@ SteadyState/Time-Dependent
  Modus=4
  Modus=1
@ Geometrie
  Geometry=1
  USERFUNCTION_YN = 1
@ MISCALLANEOUS_YN =1
  transportxs_yn=1
  dortdiffusion_yn=20
  Buckling_YN=1
  DecayHeatModel_YN=1
  LocalXenon_YN=0
  Stabilization_YN=1
@ KINETICS_YN=1
  Feedback=4
end
@Material 1 represent all the reflector regions (top, bottom, and two side reflectors made of graphite)
@Material 2 represent the fuel regions
@Material 3 is the central graphite column
@Material 4 is the mixing zone (fuel admixed to graphite at 50/50 )
@Material 5 is the control region (Boron 10)
@Material 6 is the extreme side reflector made of carbon
@Material 7 is the void region (cavity at the top of the pebble-bed) filled with Helium

BLOCK2
@
@ Number of Energy Groups   Number of XS per Group   Number of Materials in XSLIB
NumberGroups=2           NumberXS=20              NumberMaterials=190
@ Scattering Order   Position Total XS   Position Scatter XS
Scattering=0       PosSigmaTot=17        PosSigmaScat=19
PosSigmaFiss=3     PosFissionSpec=0   Possigmatrans=1
POSSIGMAKAPPA=14
POSXENYIELD = 7
POSIODYIELD = 6
POSMICXEN = 5
POSDENSXEN = 0
POSSIGMAINVVEL = 4
@POSSIGMABETA1 = 8
@
@ Boundary Conditions left/right/top/bottom
  BoundaryConditions  1 0 0 0
@
@ Prompt Fission Spectrum
PromptFission
  1.0 0.0
@end

BLOCK3
@
@ Coarse Meshes in X/R-Direction
CoarseMeshes1
  0.0000
  10.00 41.00  73.60  80.55  92.05  99.0 100.00 108.5
  117.000 125.5 134.00 142.5 151.00 159.5 168.00
  176.5 185.00 186.0 192.95 204.45 211.40 225.00 243.600
  260.60 275.00 287.50 292.5
@ Number of Fine Meshes Per X/R-Coarse Mesh

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@ Coarse Meshes in Y/Z-Direction

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<td>900.0</td>
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<tr>
<td>1200.0</td>
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@ Number of Fine Meshes Per Y/Z-Coarse Mesh

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@ Material Map for all Coarse Mesh Regions

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<td>152 152 152 189 190</td>
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<td>133 133 133 155 116 116 111 111 111 111 111 111 111 111 111 135 135 165 144 144</td>
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<td>152 152 152 189 190</td>
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<tr>
<td>134 134 134 125 156 117 117 11 1 23 23 45 45 67 67 89 89 136 136 166 145 145</td>
</tr>
<tr>
<td>153 153 153 189 190</td>
</tr>
<tr>
<td>134 134 134 125 156 117 117 2 2 24 24 46 46 68 68 90 90 136 136 167 145 145</td>
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<td>153 153 153 189 190</td>
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<tr>
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<td>134 134 134 128 159 120 120 10 10 32 32 54 54 76 76 98 98 139 139 175 148 148</td>
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<tr>
<td>134 134 134 128 159 120 120 11 11 33 33 55 55 77 77 99 99 139 139 176 148 148</td>
</tr>
<tr>
<td>153 153 153 189 190</td>
</tr>
</tbody>
</table>
UseBetaEff 0 BetaEff 0.0057218422

@ Relative Delayed Neutron Fractions, evaluated from coupled transport calculations with adjoint weighting
Beta_i
0.0232425278 0.1392993231 0.3917016352 0.1966675585 0.2054585055 0.0436304500

@ Delayed Neutron Inverse Lifetimes
Lambda_i
0.01272 0.03174 0.1160 0.3110 1.4000 3.8700

DelayedFission1
1.0 0.0

DelayedFission2
1.0 0.0

DelayedFission3
1.0 0.0

DelayedFission4
1.0 0.0

DelayedFission5
1.0 0.0

DelayedFission6
1.0 0.0

@ Energy Boundaries for Delayed Fission Spectrum Evaluation
EnergyBoundaries 2e5 1.11090E5 0.000001

end

BLOCK5

@ FRM-II Variables
@ Coarse Mesh Grid for Uncontrolled Part
CR_uncontrolled
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 164

@ Coarse Mesh Grid for Controlled Part
CR_controlled
0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 188
@ Steady State Power (kW)
SS_Power  400000.0

@ Initial Control Rod Position
CR_Position  150.0

@ K-eff Search Value for FRM-II
CR_SearchValue  1.000

@ FRM2 Rod Model
Rod_Model=3
SEARCHKEFF=0

@Controlled_Uncontrolled_Offset = -20
@CR_TIME=  0.0 1.0 1.0001 1.099 1.1 1000.0
@CR_TIME=  0.0 0.1 0.1001 0.199 0.2 1000.0
@CR_VELOCITY=0.0 0.0 -4.0  -4.0  0.0  0.0
@CR_VELOCITY=0.0 0.0 -0.0  -0.0  0.0  0.0
@CR_VELOCITY=0.0 0.0 -1323.7 -1323.7  0.0  0.0
@CR_VELOCITY=0.0 0.0 -2000.0 -2000.0  0.0  0.0
@CR_VELOCITY=0.0 0.0 -1735.4 -1735.3  0.0  0.0
@CR_VELOCITY=0.0 0.0 -1489.2 -1489.2  0.0  0.0
end

BLOCK6
@
@ Velocity Dependent Variables
@ Using Group or Zonewise Velocities?
GroupOrZone  1
@ GroupWise Velocities
Velocities
   2.125191E+07
   4.740743E+05
@
end

BLOCK7
FastIterations  20
ThermalIterations  20
ThermalLoops  1
Keff-Flux-Convergence 1e-7
Keff-EV-Convergence 1e-7
Keff-Fission-Convergence 1e-7
Chebychev 4
ChebycycleLength=5
Extrapol-Modus=1
Extrapol-Tolerance=0.2
end

BLOCK8
@ Number of Flux Moments   Number of Angular Fluxes
NoMoments 1              NoQuad 4
WhichQuad=1   DORTMODUS=0
DORTCOARSEMESH1
  0.0000  10.00  41.00  73.60  80.55  92.05  100.00
  117.000 134.0000 151.00 168.00 185.00 192.95 204.45
  211.4000 225.0000 243.60 260.60 275.00 287.50 292.5

DORTCOARSEMESH2
-200.0
-150.0  -100.0  -50.0
  0.0    50.0    100.0
150.0    200.0    250.0
300.0    350.0    400.0
450.0    500.0    550.0
600.0    650.0    700.0
750.0    800.0    850.0
900.0    950.0   1000.0
1050.0   1100.0   1150.0
1200.0   1250.0   1251.0

DORTLOCOBJ = 10000
@DORTFLXMIN=1e-25
end
@ HTR: DORT/THERMIX-Coupling Parameters

WhichLibrarySet=7

@ Radial Mesh Divisions

RadialAthlet 0.0 275.0

RadialAthletMeshes
2 2 4 4 8 2 4 4 1
4 4 4 4 4 4 4 4 4 4
1 4 4 4 2 2 4 4 4

Number_TH 190

AthletMeshes
-200.0
-150.0 -100.0 -50.0
0.0 50.0 100.0
150.0 200.0 250.0
300.0 350.0 400.0
450.0 500.0 550.0
600.0 650.0 700.0
750.0 800.0 850.0
900.0 950.0 1000.0
1050.0 1100.0 1150.0
1200.0 1250.0

RADIALTHERMIXPOWERMESH

100.0 117.0 134.0 151.0
168.0 185.0

AXIALTHERMIXPOWERMESH

0.0
50.0 100.0 150.0 200.0 250.0 300.0 350.0
400.0 450.0 500.0 550.0 600.0 650.0 700.0
750.0 800.0 850.0 900.0 950.0 1000.0 1050.0
1100.0
MaterialIdent

@ 110 Fuel Materials

26 27 28 29 30 31 32 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47
48 49 50 51 52 53 54 55 56 57 58 59 60 61 62 63 64 65 66 67 68 69
70 71 72 73 74 75 76 77 78 79 80 81 82 83 84 85 86 87 88 89 90 91
92 93 94 95 96 97 98 99 100 101 102 103 104 105 106 107 108 109 110 111 112 113
114 115

@ 1 Void Material

4

@ 52 Graphite Materials

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1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1
1 1 1 1 1 1 1 1 1 1 1
1 1

@ 25 Control Rod Mateirals

2 2 2 2 2 1 1 1 1
1 1 1 1 1 1 1 1
1 1 1 1

@ 1 Void Material

5

@ 1 Carbon Material

3

MaterialOnLibs 115

CoolantTemperatureOnLibs
300.0 800.0 1400.0 2400.0

VoidOnLibs
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FuelTemperatureOnLibs
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InterpolModus=0
T-standard=1200.0
V-standard=1200.0
B-standard=3.9E-11
Convert-YN=0
PVMXS\_YN=0
NO\_NTH\_ITER = 5
WriteModus=0
end

BLOCK10
@MAX\_TIMESTEP 10.0
TRUNCATION\_FACTOR = 100.0
MAXSTEP\_TIME 0.0 1.0 432.0 21600.0 22032.0 86400.0 1000000.0
MAXSTEP\_STEP 0.03 0.03 2.0 0.03 2.0 0.03 0.1
@MAXSTEP\_STEP 1.00 1.00 1.00 1.00 1.00 0.01 0.1
@EventTime 1.0
@EventStep 0.00001
MAXPROBLEM\_TIME = 86400.0
SCRAMTIME = 100000.0
MIN\_ITERATIONS=5
MAX\_ITERATIONS=20
END

BLOCK11
@MIXING\_MATERIALS 71
@MIXING\_CONCENTRATIONS 1.0
@DUMMY\_MATERIALS 73
END
APPENDIX B
EXAMPLE OF THERMIX-DIREKT INPUT FILE - STEADY-STATE

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<tr>
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<tr>
<td>1.0 38</td>
</tr>
<tr>
<td>20 1 41 1 38 ! top boundary</td>
</tr>
<tr>
<td>19 39 41 1 37 ! bottom boundary</td>
</tr>
<tr>
<td>21 1 41 37 38 ! side boundary</td>
</tr>
<tr>
<td>7 3 4 1 31 ! top barrel</td>
</tr>
<tr>
<td>5 4 38 1 10 ! central reflector</td>
</tr>
<tr>
<td>4 4 38 10 29 ! side reflector</td>
</tr>
<tr>
<td>3 4 7 10 20 ! top reflector</td>
</tr>
<tr>
<td>2 7 8 10 20 ! top void</td>
</tr>
<tr>
<td>1 8 30 10 20 ! CORE</td>
</tr>
<tr>
<td>17 30 35 10 20 ! bottom reflector</td>
</tr>
<tr>
<td>18 35 36 10 20 ! bottom plenum</td>
</tr>
<tr>
<td>6 36 38 10 20 ! graphite(bottom)</td>
</tr>
<tr>
<td>8 38 39 1 37 ! bottom barrel</td>
</tr>
<tr>
<td>14 33 34 27 28 ! inlet plenum</td>
</tr>
<tr>
<td>15 9 33 27 28 ! helium flow channel</td>
</tr>
<tr>
<td>16 8 9 20 28 ! upper plenum</td>
</tr>
<tr>
<td>9 4 38 29 30 ! helium gap</td>
</tr>
<tr>
<td>10 4 38 30 31 ! side barrel plate</td>
</tr>
<tr>
<td>11 3 39 31 32 ! helium gap</td>
</tr>
<tr>
<td>12 3 39 32 33 ! RPV</td>
</tr>
<tr>
<td></td>
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| 5  | 6.0  | 0.0  |
| 4  | 5.0  | 1.0  |
| 3  | 3.50 | 1.0  |
| 2  | 1.25 | 1.0  |
| 1  | 0.05 | 1.0  |

cavity 2 0 0.003 500. 1.000 -g01 0.8 00
refftop 3 0 0.200 500. 1.000 3.02
reffout 4 0 0.200 500. 1.000 3.02
refcn 5 0 0.200 500. 1.000 3.02
grpbot 6 0 0.200 500. 1.000 3.02
barrel 7 0 0.170 500. 1.0004.212
platen 8 0 0.170 500. 1.0004.212
helium 9 0 0.003 500. 1.000 -g01 0.8 11
plateb 10 0 0.170 500. 1.0004.212
helmr 11 0 0.003 500. 1.000 -g01 0.8 11
rpv 12 0 0.380 300. 1.0004.095
airout 13 0 0.0003 500. 1.000 -g02 0.8 01
plnin 14-1 0.200 500. 0.800 3.02 | 0.8 00 |
flowch 15-1 0.200 500. 0.800 3.02 | 0.8 00 |
pln 16-1 0.200 500. 0.800 3.02 | 0.8 00 |
reffbot 17-1 0.200 500. 0.800 3.02 |
plnbot 18-1 0.200 500. 0.800 3.02 | 0.8 00 |
bdrbot 19 0 1.e-30 500. 1.000 3.02 |
bdr 20 0 1.e-30 500. 1.000 3.02 |
bdr 21 0 0.8e+00 20. 1.000 |

<table>
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1100.0
5 100.
117.0 134.0 151.0 168.0 185.0
0

*** PBMR-400(DIREKT)

1.0 1.0 1.0

90.0 0 1 1
37 37 8 -235.0 0.0
35.00 2 50.00 36 35.00 37
5.00 3 15.50 5 32.60 6 6.95 7 11.50 8 6.95 9 1.0 10
8.50 20 1.00 21 6.95 22 11.50 23 6.95 24 6.80 26 18.6 27
17.00 28 14.40 29 12.50 30 5.0 31 17.5 32 18.0 33 33.5 37
3 1 37 1 37 ! no flow
2 5 6 10 20 ! top void (cavity)
1 6 28 10 20 ! CORE
4 31 32 27 28 ! inlet plenum (thx no = 14)
5 7 31 27 28 ! helium flow channel(thx no = 15)
6 6 7 20 28 ! upper plenum(thx no = 16)
7 28 33 10 20 ! bottom reflector(thx no = 17)
8 33 34 10 20 ! bottom plenum(thx no = 18)

1 0 1 0.390 6.00 ! CORE
2 1 5 1.000170.0 ! CAVITY
3 1 0 ! SOLID, no flow
4 0 5 0.200 33.5 0 192.7 500.0 ! INLET PLN.
5 0 2 0.00 0.00 0.200 17.0 ! HELIUM FLOW
6 0 5 0.200 33.5 ! UPPER PLN.
Bismark Mzubanzi Tyobeka was born on 04 November 1974 in Rustenburg, South Africa. He completed his bachelor’s degree in Physics and Chemistry in 1998 at the University of North-West, South Africa, whereupon he proceeded to complete a master’s degree in applied radiation science and technology in 2001. He was employed by Eskom Enterprises in November 2000 as a reactor physicist and in the 2002 he was seconded to Pennsylvania State University. He completed a master’s degree in nuclear engineering in 2004 and went on to study for a PhD which culminated into this thesis. His research interests are reactor physics, with special focus on coupled neutronics/thermal-hydraulics codes and methods development. He is married to Ngeniswa and together they are blessed with two daughters, Siviwe and Andiswa.