Coupled Neutronic Thermal Fluid Dynamic Modelling of a Very High Temperature Reactor

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Declaration

I herewith certify that all material in this dissertation which is not my own work has been properly acknowledged.

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Abstract

The Very High Temperature Reactor (VHTR) is designed to push the boundaries and capabilities of existing High Temperature Gas Reactor technology to higher levels, challenging the desired inherent and passive safety features. To ascertain the viability of the design requires a detailed understanding of the complex multiphysics within the reactor core and the associated energy removal system. Due to the scale of the calculation computational numerical models are utilised. During a transient the greatest challenge to inherent and passive safety design features will occur. To understand the core dynamics during these off normal conditions requires the use and development of coupled radiation transport thermal hydraulic codes.

In this thesis the coupled radiation transport computational multiphase fluid dynamic FETCH model is applied to a generic block type VHTR. The purpose of this research is twofold. First to analyse the suitability of the FETCH model to be capable of capturing the physics inherent within the generic VHTR of interest. Secondly to analyse the suitability of the generic VHTR to operate within certain key safety constraints of interest. A necessary component of this research was to provide evidence to support the reliability and credibility of model solutions through the use of a continuous verification and validation automated framework.

Also this PhD thesis includes the development and analysis of a Sub Grid Scale finite element methodology applied in the context of the multigroup neutron diffusion equations. The method was found to be superior to standard Continuous Galerkin finite element methods but suffered from stability issues associated with low, or zero, absorption coefficient terms.
Dedicated to the The Tollit Wolfpack: Zoe, Alexander and Daniel, bring it on!
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Chapter 1

INTRODUCTION

Synopsis

Nuclear energy is discussed in the context of growing world energy demand. The Generation IV international research program is described with an outline of the six selected generic reactor designs and desired characteristics used to select them. Next the Very High Temperature Reactor is presented in more detail. This includes the intended purpose, historical evolution, advantages and disadvantages as well as a comparison between the two variants being pebble bed and prismatic block. Finally, the overall purpose of this thesis is described and an outline of the chapters that follow is presented.
1.1. Generation IV Nuclear Reactors

As the world’s population increases the demand for a sustainable and reliable energy supply will rapidly increase. Combined with the ever increasing desire by many developing nations citizens for an improved quality of life, this will severely challenge the current global energy production infrastructure. Also it has become generally accepted through scientific research, as well as becoming a high profile general public and political concern, that the current energy mix (dominated through burning hydrocarbons) is contributing to the continuously changing global climate. Thus the entire populated world is facing a challenging energy supply problem in the near future. All possibilities need to be evaluated with a strong emphasis on practical and technologically realistic solutions. The future energy solution must provide an environmentally clean energy mix as well as being safe, reliable, sustainable and globally economically viable. Sustainability is important such that a secure energy supply exists for all future generations. Energy must be produced safely in an environmentally manner such that any resulting consequences on the surrounding climate (both locally and globally) are minimised. Future energy challenges will affect all nations including the United Kingdom where recent government reports DTI (2006) assess the issue and current possibilities, including nuclear rebuild.

Energy is produced and consumed worldwide for a variety of reasons such as electricity, transportation and industrial applications. A significant proportion of the current global electricity mix is supplied via commercial nuclear power. The first man-made self sustaining (critical) nuclear chain reaction occurred at the University of Chicago (United States) in 1942, led
by Enrico Fermi. Within 10 years of this historical event the first nuclear reactor power plant was built to produce electricity (the EBR-1 experimental breeder reactor in the US). Commercial nuclear power was first utilized around 50 years ago by the Calder Hall (now known as a MAGNOX Reactor) nuclear power plant at Sellafield (UK) in 1956, closely followed by various different designs in the US and former Soviet Union. The industry has rapidly matured into a valuable and reliable energy source for many nations. Currently there are over 400 commercial nuclear reactors worldwide providing around 16% of the world's electricity needs.

However, as with all base load electricity generation plants, individual nuclear reactors cannot operate for an indefinite period. Within the next few decades many of the existing commercial nuclear reactors will move into the decommissioning phase of their plant life cycle. This poses the concern for some nations as to what will replace these ageing power stations in their energy mix. Major factors influencing this decision are not solely centred on environmental concerns but also include social, political and economic factors. An important issue concerns being too reliant on high air polluting resources such as coal, oil and gas. These resources may also suffer from volatile market fuel prices due to the majority of the world's reserves being located in, what are considered by the main consumer nations, politically unstable regions. Methods to capture and store these pollutants are being researched, but these will have to prove their long term effectiveness, reliability and economic capability. Known world reserves of these hydrocarbon resources are also estimated to be diminishing rapidly at the current consumption rate. Current renewable energy sources have great potential to expand and fulfil part of the world's energy needs, with much current interest focused on micro generation. However, it is not expected that renewable energy is capable of supplying all, or a significantly large proportion, of the world's base-load energy needs. This is primarily due to them being unreliable and relatively expensive compared to other available methods. An exception is hydroelectricity but this can only be utilised where geological conditions are suitable.

As part of the future energy solution the option of new nuclear energy build needs to be considered. Realising this 10 nations (Argentina, Brazil, Canada, France, Japan, Republic of Korea, Republic of South Africa, Switzerland, UK and the US) formed an international consortium called Generation 3
IV (GenIV) to provide future nuclear reactor designs Forum (2002b). To succeed in keeping nuclear an option the entire nuclear process (not just core design) from fuel fabrication to decommissioning will be researched and optimised. The research will focus on improving the sustainability, economic, safety, reliability and proliferation resistance of novel reactor designs. These new nuclear reactor designs are based on innovative and evolutionary ideas. The potential to use nuclear power for other energy needs (not just electricity production) such as hydrogen production, industrial process heat applications, district heating and desalination will also be investigated within the consortium. As part of this process six concepts were short-listed as the most viable candidates.

The GenIV program aims to provide new alternatives to future world energy demands by the development of evolutionary and advanced nuclear reactor designs. The main goals of the Gen IV program are Forum (2002b):

1. **Sustainability** For a system to be sustainable it must cater for the present while ensuring the option for indefinite use into the future exists. GenIV nuclear reactors will be designed such that they provide a sustainable energy source that minimise the amount of radioactive waste and other harmful environmental pollutants. The new designs will incorporate improved fuel cycles incorporating higher burnup and actinide burning to improve long term waste management. The potential for significant benefits that arise from the recycling of spent fuel and the conversion of fertile material to fissile will be an essential feature for many of the new designs. This will allow for a more efficient use of fuel resources and minimise the volume of radioactive waste produced, hence reducing the physical storage space needed in geological repositories.

2. **Economics** GenIV nuclear reactors must be able to compete on the global (nationally and internationally) energy market by providing cost competitive energy. This will enable them to be an alternative attractive option to the current most common base load (coal, oil and gas) energy generation options, as well as current established nuclear power technology. An important point in this respect is that nuclear power benefits from low fuel costs and a high security of supply due to the global location of reserves compared with conventional hydrocarbon
global resources. For economic competitiveness to be achievable novel ideas such as modular designs, improved fuel cycle efficiency and reduction in the complexity of plant layout will be incorporated into new designs. The move from large scale generation plants of the 3000MWth range (consistent with many of the current commercial nuclear reactors) to small scale modular designs of the 600MWth capacity range will have the benefit of making them more accessible to developing nations, that do not contain the infrastructure to support the larger current generation plants. Modular designs will also reduce upfront capital costs and the financial risk associated with construction.

3. **Safety and Reliability** GenIV nuclear reactors will utilise advanced safety mechanisms thereby further decreasing the, already extremely low, probability of public exposure to radiological hazards. Many of these novel safety mechanisms will be passively asserted (for example due to gravity or radiative heat transfer) or be inherently part of the design concept due to the physical processes involved like a large negative temperature coefficient of reactivity. This will extend the time before human intervention in an accident scenario becomes a necessity, thus allowing operators a wider time frame to fully assess a situation before taking appropriate action (as it is often the human factor that is the most unpredictable and dangerous). Potentially this may reduce the need for off site emergency operations and regulatory restrictions on the location of nuclear plants, thus allowing them to be constructed nearer populated areas and industrial sites. Also the philosophy of Defence-in-Depth will be, as is in current commercial reactors, embodied into GenIV designs to ensure safe operation under all circumstances.

4. **Proliferation Resistance and Physical Protection** GenIV nuclear reactors will be designed such that they are an undesirable option for the diversion (or theft) of weapons grade materials. Some designs will use a closed fuel cycle allowing the use of plutonium, as well as other transuranics, for peaceful energy generating means. They will also have increased protection against disaster scenarios such as earthquakes and terrorism.
All of the proposed GenIV concepts are aimed for commercial deployment within the next few decades. Figure 1.1 shows a brief outline of the time scales associated with past, present and future nuclear reactor development. The current commercial nuclear market is dominated by the Light Water Reactor (LWR), mainly due its popularity in the U.S.A., France, Japan and South Korea. Many of the nuclear reactors due for decommissioning (mainly Generation II designs) within in the next few decades could potentially be replaced with GenIII(+) concepts, such as Westinghouse’s AP1000 or the European Pressurised Reactor (EPR). With a vast technology base, along with many safe and reliable operational years of experience, these new advanced LWR’s will be the most attractive new nuclear build option in the near future. Thus the GenIV concepts will therefore have to show a superior economic advantage compared to current GenIII and near future GenIII+ designs. Without this advantage energy generators are unlikely to invest in an unproven technology.

The GenIV program has short-listed (from a selection process of over 100 concepts) six generic nuclear reactor designs believed to satisfy with the objectives stated above. Many are multi-purpose designs that can not only be used for electricity generation but also for other industrial applications, such
as hydrogen production from the process heat generated within the reactor.

The six proposed designs (in no specific order) with a short description are:

1. **Gas Cooled Fast Reactor System (GFR)** The GFR utilises a fast neutron spectrum along with a closed fuel cycle. It will be an efficient actinide burner and capable of converting fertile resources into fissile. The proposed design will be helium cooled with an outlet temperature of 850 °C and have an operating power of 600 MWth/288MWe. The thermal conversion system will use a direct Brayton cycle for high thermal efficiency. Various fuel/clad material and assembly configurations are being considered for the retention of fission products at sustained high temperatures and prolonged irradiation exposure. It will primarily be built for the production of electricity and for actinide management, with the possibility to support hydrogen production.

2. **Lead Cooled Fast Reactor System (LFR)** The LFR will also utilize the fast neutron spectrum along with a closed fuel cycle, also capable of conversion of fertile uranium. As the name suggests the LFR will be a liquid metal cooled reactor. A range of operating powers has been suggested from small scale "battery" reactors with a power output of 50-100MWe to a large scale plant with a comparable power output with present day commercial reactors. The core of the reactor will be cooled by natural circulation, an inherent safety aspect. The LFR will be capable of electricity production, hydrogen production and actinide management.

3. **Molten Salt Reactor System (MSR)** The MSR will harness the epithermal to thermal neutron energy spectrum with a closed fuel spectrum. Molten salt will be used as a coolant and the proposed design will have an operating power of 1000MWth, working at a low pressure with an outlet temperature of 700 °C. The fuel will circulate through a graphite core in liquid form, thus reducing the need for fuel fabrication. It will be highly efficient in waste burndown. The main objectives for this reactor will be electricity generation and waste burndown.

4. **Sodium Cooled Fast Reactor System (SFR)** The SFR will operate similarly to the LFR working with a fast neutron spectrum and a closed fuel cycle. Two operating powers consisting of a medium size
plant of 150-500MWth and a larger 500-1500MWth have been proposed. Different fuel compositions are being analysed for each design (zirconium metal and oxide fuel). It is considered to be the most near term deployable actinide management reactor proposed. The SFR will be capable of electricity generation and actinide management.

5. Supercritical Water Cooled Reactor System (SCWR) The SCWR will be capable of operating using an open thermal or closed fast neutron energy spectrum. Both designs will use water, at the thermodynamic critical point (22.1MPa, 373 °C) as a coolant to achieve a thermal efficiency of roughly 44%. For both designs the operating power will be 1700MWth at a high pressure of 25MPa. The SCWR will mainly be built for electricity production.

6. Very High Temperature Reactor System (VHTR) The VHTR will use a thermal neutron spectrum on an open fuel cycle. The proposed reactor will have an operating power of 600MWth with a helium cooled core. The core design can be either prismatic fuel block or pebble bed form. Outlet temperatures will exceed 1000 °C making it an attractive heat source for many industrial processes such as hydrogen production. The primary purpose for the VHTR will be hydrogen production but it will also adaptable to co-generate electricity.

Of the six designs short-listed the VHTR is believed to be the nearest commercially deployable and is receiving increased interest in the US DOE (2001) for hydrogen production. In the next section the VHTR will be introduced in more detail.

1.2. The Very High Temperature Reactor

The VHTR can be regarded as an evolutionary development (rather than innovative) of past and present High-Temperature Gas Cooled Reactors (HTGR) Brey (2004). The HTGR is not a recent design invention. A pebble bed reactor HTGR was first proposed in 1944 by F. Daniels of the University of Chicago Lohnert (2003), making the design one of the first nuclear reactor concepts considered. Daniel’s design consisted of a homogeneous mix of fuel and graphite pebbles, 5cm in diameter, stacked 11m high and cooled by helium flowing through the core. The helium coolant was proposed to have an
The reactor was designed for the production of weapons grade plutonium (making it classified) by designing the pebbles such that plutonium leaches out into the helium from which it could be extracted. Commercial interest in the HTGR developed in the 1950’s to attain higher efficiency from Gas Cooled Reactor (GCR) designs.

The first nuclear power reactors were GCR’s and have been deployed commercially mainly in the U.K., having operated 26 MAGNOX and 14 AGR reactors. The MAGNOX (Magnesium non-oxidising) GCR used natural uranium metal fuel clad in magnesium alloy cans surrounded by graphite bricks (that acted as the moderator) and a steel pressure vessel (RPV). MAGNOX reactors had a characteristic low burnup and low power density of 1 MW/m³ and were designed for on-line refuelling. They could only achieve a cycle thermal efficiency of 25-35% due to a low outlet coolant (carbon dioxide) temperature of 370 °C. The Advanced Gas Reactor was a development of the MAGNOX reactor with an increased outlet gas (carbon dioxide) temperature of around 600 °C, thus increasing the cycle efficiency to 40%. Further increases were limited due to the possibility of chemical reactions occurring between the carbon dioxide and internal structural components at higher temperatures. The AGR used steel clad, slightly enriched uranium dioxide (UO₂) fuel pellets and a Prestressed Concrete Pressure Vessel (PCPV) allowing for a larger power, burnup and coolant pressure compared to MAGNOX designs.

The HTGR design arose for the possibility of utilising a nuclear process heat source of 900 °C or higher for industrial applications and more efficient electricity generation. To achieve this many current HTGR designs use a graphite moderated, helium cooled core with ceramic (dioxide or carbide) fuel that has multiple coatings to retain fission products. Generally the fuel is embedded in a graphite matrix of prismatic blocks or spherical pebbles. Helium is used as the primary coolant such that higher outlet temperatures are possible due to helium being chemically and neutronically inert. Although it is briefly mentioned here that research into carbon dioxide cooled medium temperature gas reactors continues to be investigated, where overall plant efficiency is compared to helium cooled counterparts. It is shown in Kato et al. (2004) that similar plant efficiencies can be achieved.
for a CO2 cooled core with lower outlet temperatures of 650 °C. This lower temperature would alleviate the requirement for advanced high temperature materials and increase safety margins related to exceeding fuel temperatures. However, the use of CO2 coolant with a graphite core is known to cause unwanted chemical reactions from extensive years of operation with MAGNOX and AGR’s.

The first HTGR built was the prototype materials test reactor Dragon \cite{Simon2002} in the UK which achieved first power in 1965. The Dragon reactor was graphite moderated, helium cooled, with the core contained within a steel pressure vessel and using highly enriched UO$_2$ TRISO (Triple-Isotropic) coated fuel particles. Dragon had an outlet helium temperature of 750 °C and a power output of 20MWt. TRISO fuel particles shown in figure 1.2 consist of small kernels (around 200-800 µm in diameter) of ceramic fuel (fissile, fissionable or fertile) coated in a layer of porous carbon (for fission gases to expand into), then three coating (hence "TRI") layers of carbon. These three layers are one inner and one outer layer of pyrolytic carbon and one middle layer of silicon carbide. These coatings act as a mini pressure vessel around the fuel kernel and are intended to prevent the release of fission products into the primary circuit of the reactor. TRISO fuel particles have been shown to retain structural integrity under high temperatures and burnup of fuel characteristic of the conditions expected in HTGR’s \cite{Nickel2002}.
Dragon was originally designed with fission product (FP) emitting fuel with an associated helium purification and FP removal system. This was shown to be highly effective in stopping FP’s dispersing through the entire primary system. The design later changed to use FP retention fuel to allow easier maintenance to the primary system. The Dragon reactor program demonstrated the development and fabrication of the TRISO particles as well as their ability to retain FP’s up to a fuel temperature of 1200 °C. Dragon provided valuable information on the behaviour of graphite and helium at high temperatures and demonstrated the ability to control core power via the coolant flow rate Simon and Capp (2002). Following from this prototype a 1320 MWe HTGR was proposed in the U.K. but the idea was abandoned in favour of a heavy water reactor concept, which itself was never commercialised.

The Arbeitsgemeinschaft Versuchsreaktar (AVR) HTGR achieved first criticality in 1965 in Germany. The AVR Pohl (2006) was the first pebble bed HTGR constructed which had an helium coolant outlet temperature of initially 850 °C, but was later raised to 950 °C. The AVR had a cylindrical core consisting of mixed fuel (with embedded TRISO UO₂ particles) and graphite (moderator) pebbles with a power of 46MWt/15MWe. The AVR used an on-line refuelling system where pebbles were continuously recirculated through the core until the desired burnup had been achieved. The AVR operated successfully for 21 years and was shut down due to lack of funding.

The first HTGR in the U.S.A. was the Peach Bottom Unit 1 Brey (2004) that achieved first criticality in 1965 and began commercial operation a year later. Peach Bottom used uranium carbide (UC) fuel with FP’s being vented to the helium coolant then purged in the primary circuit. The fuel kernel was originally coated with an anisotropic carbon layer. However, due to high fuel failure this was changed to a single Buffer-Isotropic (BISO) carbon coating.

Each of these prototype HTGR’s provided valuable information on the operation of a HTGR as well as the behaviour of structural materials under high temperatures and irradiation. They also provided a test bed for new fuel matrices of the multiple coated particle form and demonstrated inherent safety features of the HTGR design (such as slow thermal response during a transient). From these small power prototype HTGR’s larger power de-
signs were proposed for full scale commercial use. This accumulated in two larger demonstration HTGR’s being built in the 1970’s and 1980’s. The first was Fort St. Vrain (FSV) built in the U.S.A., which achieved first electricity generation in 1976. This was the first HTGR to use prismatic fuel blocks (hexagonal blocks) with fuel rods inserted containing TRISO particles and with a Pressurised Concrete Reactor Vessel (PCRV) rather than a steel vessel. Also, FSV used a secondary loop of water to produce superheated steam to drive a generator with an electrical power output of 330MWe. FSV suffered from significant loss of availability due to unforeseen problems associated with water lubricated bearings in the helium circuit and fuel assembly stack movements resulting in core fluctuations. Despite this FSV was valuable for verifying TRISO particle properties for retaining fission products as well as fuel handling and helium purification. The second HTGR demonstration power plant built was the Thorium High Temperature Reactor (THTR-300) in Germany during the 1970’s and 1980’s. THTR-300 was a pebble bed reactor with uranium-thorium fuel particles and an electric power of 296MWe. However, the THTR-300 suffered from a long construction period due to complicated licensing procedures and was prematurely closed due to economic reasons and increasing public concern in 1989.

The initial primary focus of HTGR’s development was to build large scale plants with a secondary indirect steam cycle for electricity production. However, due to an economic decline there was no wide commercial deployment of any HTGR design. The initial large HTGR has many attractive safety features but due to the high power still relied on active cooling systems to maintain structural temperatures below design basis limits in the unlikely event of a transient.

In the 1980’s and 1990’s, HTGR research shifted focus on to smaller modular designs Tsuchie (2000). These modular designs would be capable of cooling the core via passive means only (although this does not imply passive systems are relied on first but as a safe last resort) to limit peak temperatures in transient scenarios when primary coolant systems fail. This is achieved by limiting the core power density and shaping the reactor to aid heat removal. The first modular HTGR design was the HTR-MODULE of Siemens/Interatom Lohnert (1990) that was developed in the early 1980’s with an electric power output of 80MWe. Fundamental to the HTR-MODULE’s design was that sufficient core cooling (provided by the
Emergency Core Cooling System, ECCS) exists via passive means under all extreme accidents such that the release of fission products to the surrounding environment is minimised below the licensing regulations. The HTR-MODULE was a pebble bed reactor similar to the previous German AVR, with a small core diameter of about 3m and a power density of 3MW/m³ (small compared to current LWR power densities of around 50MW/m³). The reactor was designed such that the maximum fuel temperature remains below 1600 °C under all circumstances Kohtz and Haque (1992), as the evidence and experience gained from the two previous German HTGR’s suggest that above this value significant fission product release could occur Nickel et al. (2002).

Also in the 1980’s the U.S.A. investigated a smaller modular HTGR that came to be known as the Modular HTGR, or MHTGR. This had a prismatic annular fuel matrix core allowing power to be increased to 450MWt while still retaining passive safety criteria. The annular core enables an increase in power van Heek (1994) due to the central reflector acting as a heat sink and the short conduction length from the fuel to the RPV boundary increasing heat loss to the ECCS. It was known that plant efficiency (approaching 50%) could be achieved by changing from an indirect to a direct Brayton cycle, where the outlet coolant helium is fed directly to the turbine generator for electricity generation. However, this option is only recently becoming realistic with advances in gas turbine technology. Also recent advances in magnetic bearings (instead of water lubricated) will eliminate the potential problems that occurred in FSV reactor. For the application of nuclear process heat efficient heat exchangers are required that, again due to recent material advancements, are now a realistic design option. Partially due to these important points the small yet renowned interest was reborn in the 1990’s to design and commercially deploy HTGR’s for electricity generation and process heat applications. The two leading designs to emerge were the Pebble Bed Modular Reactor (PBMR) and the Gas Turbine Modular Helium Reactor (GT-MHR). The VHTR can be considered as the next evolutionary step up from these two designs.

The PBMR Koster et al. (2003) is being developed primarily by the South African utility company Eskom and is based on the German HTR-MODULE design from Siemens. The PBMR has an annular core of spherical fuel assemblies 6cm in diameter, within which are embedded the TRISO fuel particles.
Originally a design with a dynamic central reflector was proposed that was formed from 6cm graphite pebbles (no fuel), which became known as the PBMR268 due to the reactor power of 268MWt. The decision was then taken to change to a fixed central reflector Koster et al. (2003) such that a higher power could be achieved while still remaining within set safety margins. With a dynamic reflector there exists a mixing zone of fuel pebbles and graphite pebbles leading to a highly neutronically thermalised fuel region that would have locally a higher power density, which would limit the overall reactor power. With a fixed central reflector this cannot occur although large power peaking is still located at the fuel-reflector boundary. The latest version has a power of 400MWt/165MWe, a helium coolant outlet temperature of 900 °C and will be constructed in groups of 6 modules or more on the same nuclear island. The PBMR is in advanced stage of development (due to evolving from previous proven designs and technology) and a demonstration plant was expected within the next decade. However as of mid 2010 the majority of financial support for the PBMR program was stopped and the project has essentially halted.

A simplified outline of the PBMR plant layout is shown in figure 1.3. This shows that a recuperator is used to recover the waste heat from the turbine exhaust to heat the helium coolant before it re-enters the core. Also, this illustrates that the pre-cooler and inter-cooler act as an ultimate heat sink for over half the core thermal power. A VHTR could have a similar layout and
research is required to determine if the materials used in the recuperator and coolers can withstand the VHTR conditions Forum (2002a). An alternative power conversion system being proposed under Areva’s ANTARES VHTR project Gauthier et al. (2006) uses an indirect combined cycle as shown in figure 1.4. A few of the advantages Gauthier et al. (2006) of this approach include:

- the freedom to choose the secondary working fluid,
- the use of ‘off the shelf’ combined gas turbine technology,
- greater efficiency with a bottom Rankine cycle,
- no contamination of the electricity/process heat equipment
- and a reduced inlet temperature of 400 °C leading to a reduced risk for the reactor pressure vessel.

The GT-MHR P. and LaBar (2002) is based on the MHTGR and FSV designs and is being developed mainly in collaboration between the Governments of the U.S.A. (General Atomics) and Russia (MINATOM), with
France (Framatone ANP) and Japan (Fuji Electric) supporting. The GT-MHR also has a annular core but uses prismatic fuel assemblies with fuel rods embedded with TRISO fuel particles. The original GT-MHR is envis-aged for the utilisation (destruction) of surplus weapons grade plutonium that has accumulated from the Cold War. The core will be fuelled solely with weapons grade plutonium enabling more efficient destruction than that available from current methods, such as the use of Mixed Oxide Fuel (MOX) in current LWR’s. The reactor will have a very deep burnup of 640 MWd/kg ensuring any spent fuel is not suitable for other means proliferation related. To make the reactor inherently safe Kodochigov (2003) it is necessary to include the burnable poison Erbium to ensure a negative temperature coefficient throughout the entire life cycle. The GT-MHR will have a power of 600MWt with a helium coolant outlet temperature of 850 °C. The GT-MHR is the base design for the uranium fuelled U.S.A. V/HTR research program called Next Generation Nuclear Plant (NGNP) MacDonald and et al. (2003).

Contributing to the HTGR renaissance two more HTGR prototypes were constructed in the 1990’s. The first was the High Temperature Test Reactor (HTTR) constructed by the Japan Atomic Energy Research Institute (JAERI) that achieved first criticality in November 1998 then soon after a full power of 30MWt Shiozawa et al. (2004). The core consisted of prismatic fuel assemblies in an annular configuration using TRISO fuel particles. The HTTR is being used to test fuel performance and as a demonstration for process heat applications such as hydrogen production. The HTTR is part of JAERI’s program to develop their own commercial HTGR called the Gas Turbine High Temperature Reactor (GTHTR-300) Kunitomi et al. (2004). The second recent prototype to be built was the High Temperature Reactor Test Module (HTR-10) by China’s Institute of Nuclear Energy Technology (INET) Wu et al. (2002). This is a pebble bed reactor that achieved first criticality in late 2000 then soon after a full power of 10MWt. Again the HTR-10 is providing valuable data on irradiation behaviour and inherent safety features of the HTGR.

Many of the mentioned HTGR’s have their important design characteristics summarised in table 1.1.

The proposed VHTR design in the GenIV program has two variants, one based on previous pebble bed HTGR’s and the other on previous prismatic block HTGR’s. The VHTR would primarily be dedicated to the
Table 1.1: Basic Parameters of Past, Present and Future HTGR

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co-generation of both electricity and hydrogen. However the generation of hydrogen would be the most appealing of the two options, as hydrogen potentially has a market twice as large as electricity. The VHTR would be capable of producing 2 million cubic meters of hydrogen per day with an electricity generating efficiency greater than 50% (compared with 47% for existing HTGR’s and just over 30% for existing commercial reactors like LWR’s). Hydrogen may be produced from the high temperatures of the reactor coolant via two methods. These are the Iodine/Sulfur Thermo-chemical Cycle and the High Temperature Electrolysis process, although these are still an active research area. The excess heat generated could also be used for other industrial processes such as those found in refineries for upgrading crude oil as well as in the production of Steel, Aluminiun Oxide and Aluminium. Other uses of the process heat include local district heating and desalination. The current VHTR design would use a once through fuel cycle of low enriched uranium.

Although the VHTR design is based on well researched HTGR designs, because it represents another evolutionary step there is still the need for further research into all design aspects Forum (2002a). Of particular interest is how to obtain the higher temperatures while remaining inherently and passively safe and what effect these higher temperatures will have on the reactor materials properties. For example the TRISO fuel particles were initially proposed for utilization in the VHTR, however these have been optimised for use under HTGR conditions. The TRISO fuel particles have been shown to retain fission products below 1600°C, so the VHTR must be shown to limit maximum fuel temperatures below this crucial value if using conventional HTGR TRISO particles. However, it is known that during normal operation certain fission products attack the TRISO coatings and gradually diffuse through. Of main concern are Silver, Caesium and Palladium at high temperature and burnup. The release of these fission products to the primary system should be limited to allow easier maintenance operations on the gas turbine (for the PBMR the bench line temperature for significant silver release was found to be 1130 °C Køster et al. (2003)). Therefore new coating techniques have already been suggested by using materials such as Zirconium-carbide (ZrC) Minato (2000) as a coating in place of the Silicon-carbide layer (nicknamed TRIZO). This idea has been shown to be superior to the conventional TRISO but it is known that ZrC oxidises more readily.
if the fuel kernel is uranium dioxide, which is the most common fuel form used currently. A solution to this would be to use uranium carbide fuel kernels (used in previous HTGR’s) but further research is also required to validate this combination of the two materials. More research is also required to find materials (available or new) for the core support structures, as the failure of these could determine the maximum outlet helium temperature with a downward flowing coolant. The choice of materials for all design components relies on the knowledge of the reactors neutronic and thermal hydraulic conditions during normal and off normal states, which is gained through experimental and computational mathematical modelling.

In the next section the main advantages and disadvantages of the generic VHTR are summarised.

1.2.1. VHTR Advantages and Disadvantages

In this section the main advantages and disadvantages of the VHTR Forum (2002a) are summarised. The main advantages of the VHTR can be summarised as:

1. Higher fuel burn up (200 GWd/t) compared to current LWR (50 GWd/t) reactors thus improving fuel efficiency (but not as high as the proposed GenIV Molten Salt Reactor) and producing less heavy metal radioactive waste.

2. An overall negative temperature coefficient of reactivity providing an inherent shut down mechanism in the unlikely event of a transient.

3. The large volume of graphite forms a heat sink and causes a large thermal inertia. This will aid in reducing maximum temperatures and slow down reactor changes during a transient. This allows for there to be no definite reliance on active safety systems immediately during a accident. An annular core increases this volume of graphite causing further reductions and allowing an overall power increase.

4. The use of helium as coolant which is chemically and neutronically inert (although small impurities of $^3$He will be present as well as trace amounts of other gases) that remains single phase under all operating conditions. This implies a more predictable heat transfer coefficient than the two phase conditions experienced in LWR’s.
5. A solid moderator core improving core structural stability which also
does not suffer from issues concerning phase change as found in LWR's.

6. Using a graphite moderator which has a low absorption cross section
(about 100 time less than water) improves the core neutron economy.

7. The ability to remove decay heat in an accident scenario using passive
means only (an important design constraint that limits core power)
by radiation, conduction and natural convection. As a consequence of
this a smaller exclusion zone will be required enabling the VHTR to
be located nearer to consumers (such as on an industrial site). Emer-
gency passive core cooling also simplifies plant design reducing capital
construction cost.

8. Multiple barriers to the release of fission products from the TRISO
fuel matrix (including the fuel kernel) acting as the initial containmen-
t and mini pressure vessel. This will allow easier maintenance of the gas
turbine due to the reduced contamination of the primary circuit.

9. The TRISO fuel particles have a high surface to volume ratio giving
efficient heat transfer from the fuel kernel to the surrounding graphite,
which also has a high conductivity.

10. The moderator to fuel ratio can be easily altered via varying the
TRISO particle concentration in the graphite matrix while retaining
the same geometry from a hydraulic cooling perspective. This gives
greater flexibility to design a fuel with the required reactor physics
quantities than that is capable in current LWR's (where the fuel as-
sembly geometry would have to be altered).

11. The fuel matrix is considered well suited for direct spent fuel disposal
in a geological repository. This is due to the TRISO particles ro-
bustness under a range of conditions, hence reducing the possibility of
radiological materials leaching to the surrounding environment.

12. High thermal efficiency through the use of the Direct Brayton cycle
for energy conversion to electricity and the through higher operating
temperatures.
13. A simplified modular plant design (using ideas such as coaxial piping) reducing the complexity of plant for operators and enabling factory batch production thus reducing on site construction (with its associated problems).

14. Low operation and maintenance costs making the design more economically competitive. Low maintenance costs are achieved via a replace rather than repair methodology achievable due to modular design.

15. Good proliferation resistance due to the multiple barriers in the fuel matrix and high burnup making the spent fuel unattractive for diverting to weapons programs.

16. Due to improved plant efficiency (approaching 50%) less waste heat is present in the power conversion system. Thus a smaller heat rejection system is required compared to current LWR's to the extent that water cooling is not necessarily required and heat can be directly rejected to the atmosphere. This will open the possibility for a VHTR to be built in arid regions opening up new markets.

17. The VHTR is an evolutionary design based on a proven technology base of previous and current prototype HTGR's.

18. Finally, the ability to adopt a uranium/thorium/plutonium (as well as potentially burning other actinides) fuel cycle for improved waste management which is possible due to no significant moderator void coefficient (which is a restraint for maximum MOX loading in current LWR's).

The main disadvantage of the VHTR is the proposed once through fuel cycle (including multiple passes) reducing the plant sustainability (a key requirement for GenIV). However, this could be increased by considering a symbiotic fuel cycle with another reactor such as the GFR, although initially a symbiotic cycle with LWR’s would be considered for waste burn down. Another disadvantage is that the coolant helium is expensive so leakage from the primary circuit will need to be minimised. Another disadvantage of large graphite moderated cores like a VHTR is the possibility of spatial Xenon transients which could potentially limit the height of the VHTR design. Also due to the use of dispersed fuel particles more neutrons are absorbed in the
$U^{238}$ resonances requiring a higher enrichment of 10% - 20% in comparison to LWR's.

In the next section the two basic fuel matrix designs, pebble and prismatic, will be compared illustrating the advantages of each compared to the other.

1.2.2. Prismatic Block vs Pebble Bed

V/HTGR's can generally be classified by their type of fuel assembly. Generally there are two types being:

1. prismatic fuel block type, typically with a height of about 80cm and cross width of about 36cm,

2. pebble bed fuel type, typically with a radius of around 6cm.

Both types use embedded TRISO fuel particles within the fuel matrix, but their different fuel matrix structure has influences on the operation of the reactor core. In this section the advantages and disadvantages of each type are stated for comparison.

The main advantages of a pebble bed reactor over a prismatic core Slabber (2004) are as follows:

1. Core Flexibility Pebble bed designs can be operated with flexible fuel cycles. One of the most appealing is the MEDUL cycle. This will involve continuous online refuelling with the flexibility to use various different fuel materials at the same time. For example, U-Th, Pu and MOX fuel pebbles could be used at the same time as well as having different enrichment's of $U^{235}$. Pebbles will pass through the core and are then assessed for burnup to decide whether to recirculate them or discharge them to interim storage. Online refuelling implies that no reactor shut down is required for refuelling. Two other fuel cycles are the Once-Through-Then-Out (OTTO) cycle and the Peu à Peu (PEP) cycle (little by little in French).

2. Fuel Handling Due to the reactor shut down required for refuelling, the prismatic design will reduce the effective availability of the reactor. The pebble bed reactor will only have to be shut down when reflector blocks are required to be changed.
3. **Amoeba Effect** The higher temperature gradient experienced in the prismatic design will make it more prone to the amoeba effect (movement of the fuel kernel against the temperature gradient which could result in structural failure of the fuel coating). This implies the pebble design will be safer in this respect.

4. **Economics** Pebbles can be more easily mass produced which will save production costs. The prismatic block construction may require different composite fuel blocks to compensate for excess reactivity and reduce power peaking factors as well as introducing burnable poisons and varying enrichment’s into the core.

5. **Power Conversion Efficiency** For the same fuel temperature the pebble bed design produces a higher core outlet temperature than the prismatic design, making it more efficient Slabber (2004).

6. **Fuel Utilization** Due to continuous fuelling with multiple passes through the core each pebble reaches the required burn up limit before being separated from the core fuel cycle. This allows a more efficient fuel utilization.

7. **Excess Reactivity** The continuous refuelling implies very little excess reactivity is required compared to the prismatic block design, which would require burnable poisons to compensate for this (adding complexity to the design).

8. **Hot Spots** In the pebble bed core the hottest part of the reactor will be shared by many fuel elements due to the dynamic core whereas in the prismatic core certain fuel assemblies will have to sustain prolonged exposure to these conditions.

The main advantages of a prismatic core over a pebble bed reactor are as follows:

1. **Core Structural Integrity** A prismatic core is less susceptible to unwanted sudden, or gradual movement of fuel matrices that may occur in a dynamic pebble bed core design, especially in extreme situations like earthquakes.
2. **Static Core** The temperature, helium flow and power fields are more easily predicted for a prismatic core than for a dynamic pebble bed core. In the AVR pebble bed demonstration plant experiments found temperatures to be hotter than expected perhaps due to bypass flow in control rod channels Pohl (2006).

3. **Improved Control** The prismatic core can have control rods inserted into the fuelled region allowing more control flexibility, which is not possible in a pebble bed core. Not being able to insert control rods into the core of a pebble bed inflicts another restraint on the radial size of the core, as reflector control rod worth reduces as the core radius increases.

4. **Helium Pumping Power** The pebble bed core requires a larger pumping power for the helium coolant through the core than the prismatic core due to the larger pressure drop associated with a packed bed compared to multiple channel arrangement.

5. **Coolant Geometry** The prismatic core has more control over varying the cooling geometry, such as the solid volume fraction that acts as a heat sink.

Preference for a pebble bed or a prismatic block reactor is therefore unclear. Pebble bed reactors achieve online refuelling whereas prismatic block reactors have more flexibility in controlling the core cooling geometry. It is considered that this latter point is why the prismatic design has gained an initial preference to the pebble bed to satisfy the GenIV VHTR requirements.

**1.2.3. VHTR Summary**

The VHTR is a promising next generation nuclear reactor capable of co-generation of electricity and hydrogen. It would operate on a similar basis to current HTGR prototypes using either a pebble bed or prismatic block fuel arrangement. Some advantages of using a pebble bed design over a prismatic block design and vice versa were briefly assessed. The design would take advantage of passive safety features and incorporate a defence-in-depth policy ensuring an extremely low probability of radiotoxic exposure of the
The VHTR would have an inherent negative feedback loop due to the negative temperature coefficient. This which would assist in the prevention of exceeding design limit temperatures regarding the failure of barriers against fission product release. The VHTR would incorporate passive decay heat removal (as a last resort) via reaching a compromise between natural heat removal from the RPV and neutron leakage from the core (a tall thin core improves decay heat removal but increases neutron leakage). As with current HTGR designs the VHTR would have an annular core to maximise power while retaining passive safety. The design would be based on modular construction such that whole plants can be gradually increased in size reducing upfront capital costs. The high temperatures reached (greater than 1000 °C) would require further research into materials for construction of both the reactor core structure and fuel particles, possibly using uranium carbide kernels with improved TRISO coatings. It is expected that a VHTR could be constructed by 2020, with designs based on the GT-MHR and the PBMR reactors Forum (2002b).

1.3. Thesis Purpose and Outline

The primary purpose of this thesis is to analyse the capabilities of the FEM based FETCH model to accurately simulate and make predictions of a generic block type VHTR such as to be able to draw conclusions as to the suitability of the reactor design with regard to physical responses of interest. Herein this research is solely focused on the active core region of the VHTR and not on the energy conversion system. To achieve this the rest of this thesis is structured as follows.

- In chapter 2 the coupled radiation transport thermal fluid dynamic theory is described in detail. An overview of each individual component is given followed by a literature review of coupled methodologies that have been used as tools for analysing HTR reactors. A detailed description of the methodology within the FETCH model is presented.

- Chapter 3 discusses best known methods to assert evidence to support Verification and Validation (V&V) claims with regard to the FETCH model. An overview of V&V is given followed by a description of previous V&V support evidence gathered in the past. A description
of an automated V&V framework is given and how this was applied to FETCH. A 3D multigroup FEM diffusion code that resulted from this process is presented as well as V&V test cases to support this code.

- Chapter 4 develops and applies a Sub Grid Scale FEM based methodology to the multigroup diffusion equations. The method derivation is given in detail followed by application to a range of eigenvalue problems.

- Chapter 5 introduces the generic VHTR design that is analysed. The radiation transport models developed in FETCH, WIMS9 and MONK9 are described and used to analyse the reactor design from a criticality perspective. A range of increasing complexity models are used and compared. To partially validate the WIMS9-FETCH method the IAEA Chinese HTR-10 critical height benchmark is performed. Spatial and energy convergence are investigated as well as the importance of neutron streaming. Changes to the VHTR design to reduce reactivity are presented.

- Chapter 6 describes the FLUIDITY model of the VHTR used within FETCH. This includes the development of a thermal submodelling approach to capture the homogenised heterogeneity within the whole core model. Coupled simulations of the generic block type VHTR using a control rod movement algorithm are presented. Comparisons are made between 2D RZ and 3D XYZ models. Suitability of the model and the generic reactor is discussed.

- In chapter 7 the thesis conclusions are presented with suggestions for future research.
Synopsis

The general theory involved in coupled radiation transport thermal fluid dynamic modelling of nuclear reactors is presented. Motivation for the continual progression of methods is given. The methods used to individually model radiation transport and thermal fluid dynamics are briefly discussed. Methods embodied in coupled codes applied to nuclear reactors in general and more specifically to HTGR’s are reviewed. Finally the mathematical theory involving the derivation and solution method used within the FETCH model is presented.
2.1. Introduction

For the safe operation of a nuclear reactor it is necessary to know the operational boundary conditions within which the system can operate without any unwanted consequences. Examples of this include the release of radioactive material to the surrounding environment and a reduction in load capacity due to required maintenance after any abnormal reactor behaviour. To obtain these conditions a detailed and realistic understanding of the physics occurring within the whole reactor is required. This understanding requires empirical experiment and theoretical solutions of the relevant physical equations. Because of the large number of calculations needed for a theoretical solution within the complex domain of a nuclear reactor, computational numerical simulation is widely utilised. Due to the complexity of a nuclear reactor and the relevant equations, it was customary in the past to simplify the geometry (for example by homogenising) and to approximate the equations (for example by reducing the number of dimensions) to obtain results. Therefore only conservative safety limits could be obtained in this way implying the resulting design may not be the optimal with respect to many factors such as economics or safety.
Contained within a nuclear reactor there are many physical processes occurring that can be broken down into distinct topics for analysis. These include Neutron Kinetics (NK), Thermal-Hydraulics (T-H) and Structural Mechanics (such as Fuel Performance). In the past when limited computational power was available, these topics were evaluated to obtain theoretical solutions independently of each other, or with extremely simplified models of one or more of the other areas. For example, a detailed T-H calculation would have performed with an assumed steady state core power profile or a zero dimensional NK model. In recent years with the continuing advancement in computer technology and numerical algorithms it has become possible to model more complexity allowing a more in depth understanding of nuclear reactor dynamics. These programs (or codes) are classed as Best Estimate (BE), in contrast to previous Conservative codes. Initially these BE codes (within their own areas) were developed independently of the other areas, or coupled to a conservative code of another area. It has now become desirable to couple together BE codes from each different topic to understand complex feedback occurring between each during a transient scenario. For accident analysis it has become obligatory to couple together Best Estimate NK and T-H codes to ascertain a better estimate solution of maximum power and temperature limits of a reactor design for all realistically possible scenarios (Structural Mechanic codes are not discussed as a part of this research). In the future the coupling will be extended to include other modules such as structural, fuel management and depletion codes.

In the next section a brief outline of the methodology behind NK codes is given. A similar outline is given for T-H codes in the following section. Then in the following section Coupled NK T-H codes are discussed outlining various methodologies, capabilities and applications. Following this a detailed description of the theory embedded within the FETCH code is given.

### 2.2. Neutron Kinetic Modelling

To determine the space-time dependent fission rate requires the knowledge of the neutron flux (the product of neutron density and speed) field. The space-time dependent neutron flux field is obtained from the solution of the neutron transport (or neutron diffusion) equation and associated delayed precursor concentrations (usually given by 6 pseudo groups). This is a
highly complex calculation that can only be achieved analytically for simplified scenarios and geometries, therefore requiring computational methods. Numerical solutions to the Boltzmann Neutron Transport equation Lewis and Miller (1993) can be broadly divided into two types; deterministic and Monte Carlo. The Monte Carlo method treats the neutron flux field in a Lagrangian view, with a solution gradually being formed from the summation of particle histories (the trajectory of a particle through the domain from beginning of life until death arising from being absorbed or leaking across a boundary). The method is statistically based requiring the sampling of many histories but is capable of modelling complex geometries precisely. It is widely used as a reference solution for verifying deterministic methods for reactor shielding and reactor physics. The main disadvantage of the Monte Carlo method is the long computational requirement making it impractical for use in a coupled transient code.

The deterministic approach treats the neutron flux in an Eulerian view and solves the Boltzmann equation by discretising all the variables. Although this causes numerical errors, a faster solution is obtained compared to the Monte Carlo approach. A variety of deterministic methods exist, differing predominantly in the way the angular variable is handled and the form of the Boltzmann equation used. The three main forms are the first order form, the second order (including even/odd parity) form and the integral form. The integral transport form involves integrating out the angular dependence leaving only the other dependent variables (space, energy and time) to be discretised. The integral form requires the solution of a dense matrix, rendering the method impractical for problems involving large geometric domains such as a whole reactor core. It is widely used for small scale lattice cell calculations with successfully developed methods such as the collision probability method. Lattice cell calculations are used in the generation of group constants for larger reactor physics codes and are thus essential to the whole core modelling process. A range of spatial discretisation methods have been applied to the first order Boltzmann equation including finite difference, finite volume and finite element. The angular variable can be discretised in many ways but the most popular is the discrete ordinate approach. This involves solving the angular neutron flux in a discrete number of directions. The second order form cast into an equivalent even/odd parity relation lends itself to a variational approach. This
is advantageous due to the particular resulting characteristics of the matrix equation formed (one being symmetric) allowing faster numerical algorithms. The second order form has been readily solved with a finite element Ackroyd (1995) spatial discretisation and spherical harmonic (standard angular functions) angular discretisation. To spatially approximate the second order form no consideration is necessary with regard to numerical stability for a reasonable resolution. Therefore conventional Continuous Galerkin methods are applicable. However, around the interface of rapidly changing material properties non-physical oscillations can occur for these methods which could be removed through the use of discontinuous methods. To spatially approximate the first order form stabilisation methods are needed such as SUPG Eaton (2004), Discontinuous Galerkin methods Reed and Hill (1973) or Sub Grid Scale methods Buchan et al. (2010).

While computational transport theory has become a well established research area, coupled neutronic thermal hydraulic codes rarely use these methods. Instead the neutron diffusion equation is usually solved within a few group (sometimes as few as two, with one fast and one thermal) multigroup energy formalisation. This is such that whole core solutions can be obtained within a reasonable time frame with available computational resources. The neutron diffusion equation can be derived independently in a heuristic manner or via the Boltzmann equation Duderstadt and Hamilton (1976). Essentially this derivation involves integrating the angular dependence out leaving the neutron balance equation given by

\[
\frac{1}{v} \frac{\partial \phi(r, E, t)}{\partial t} + \nabla \cdot J(r, E, t) + \Sigma_t(r, E, t) \phi(r, E, t) = \int_0^\infty dE' \Sigma_s(r; E' \rightarrow E; t) \phi(r, E, t) + S(r, E, t) \tag{2.1}
\]

where \( \phi(r, E, t) \) is the neutron flux density at position \( r \), with energy \( E \) at time \( t \). The term \( \nabla \cdot J(r, E, t) \) represents the streaming of neutrons across the domain, where \( J(r, E, t) \) is the neutron current density. The term \( \Sigma_t(r, E, t) \phi(r, E, t) \) is called the removal term where \( \Sigma_t(r, E, t) \) is the energy, spacial and time dependent total macroscopic cross section. The right hand side represents the scattering source at position \( r \) from energy \( E' \) to \( E \), plus the term \( S(r, E, t) \) which is a combination of external and fission source neutrons. To obtain the neutron diffusion equation a relation between the
two unknowns, the neutron flux density $\phi(r, E, t)$ and the neutron current density $J(r, E, t)$, given by

$$J(r, E, t) \cong -D(r, E)\nabla \phi(r, E, t)$$

(2.2)

is implemented as a constitutive closure law. This type of diffusion approximation implies that neutrons will diffuse from high density regions to lower density regions (down the gradient) and similar relations are commonly used in other areas of physics such as heat conduction. The diffusion coefficient $D(r, E)$ is obtained in the derivation from the Boltzmann equation and given by

$$D(r, E) = \frac{1}{3\Sigma_{tr}(r, E)},$$

(2.3)

where $\Sigma_{tr}(r, E)$ is the transport macroscopic cross section. Although the neutron diffusion equation is more easily solved numerically it must be understood that the approximation is invalid near highly absorbing media (such as control rods) and at material and core boundaries. However, when performing a whole core calculation a large degree of homogenisation preludes the main core calculation. This often smears the effects of rapidly changing regions over a larger region rendering a problem definition more readily applied to diffusion theory. A range of methods exist for the discretisation of the neutron diffusion equation including the classical finite difference/volume/element methods.

By far the most widely used method is the Nodal method Stacey (2007), where the term node here refers to a volume rather than a point as the word is commonly used in finite element methods. The method has become highly developed producing accurate fast solutions to whole core problems. Typically nodal methods use transverse integration such as to solve three 1D coupled equations rather than one 3D equation. The three 1D equations are coupled through a transverse leakage term that is typically approximated with a quadratic variation. To solve each 1D equation either analytic solutions or high order (fourth or fifth) Legendre polynomials are used within each node to produce a balance equation between all nodes. Nodal codes are typically restricted to geometries constructed from structured cubes or hexagonal prisms, which is the standard repeated fuel assembly geometry.
found within a nuclear reactor.

The use of coarse mesh FEM models for whole core modelling is also a possibility but would require significantly more computational work than Nodal methods. Use of higher order basis functions would achieve increased convergence rates but at the expense of a less sparse matrix system. The FEM however can readily handle more general geometries and be easily linked with FEM based CFD solvers to produce coupled whole core models. Also as computational power increases research will challenge conventional methods of the two step homogenisation method and thereby resolve more of the heterogeneity requiring a general unstructured method like the FEM.

Neutron kinetic codes are used to obtain the core criticality factor and space time power distribution. These can then be analysed to ensure they do not breach design specifications (such as linear power rating) required from a thermal hydraulic perspective. They can also be used for burnup calculations where the long term prediction of core composition is desired as it will affect the neutronic spatial distribution and determine core lifetimes between refuelling.

2.3. Thermal-Hydraulic Modelling

Determining the thermal hydraulic behaviour of a nuclear reactor under all circumstances is essential to ensure full life time safe operation and that the reactor operates in an optimal state. Many of a nuclear reactor's design limitations and operational limits are determined by thermal hydraulic considerations. The power density is limited to ensure that core materials do not exceed safe temperature limits, such as phase change values. Therefore to achieve a specific total power, with the restrained power density, the whole core size will be determined from a thermal hydraulic perspective. This itself could also be limited to ensure safe removal of decay heat during a transient. The choice of coolant and circulation characteristics (pressure and inlet temperature) is also determined partly via a thermal hydraulic analysis (as well as the neutronic effects) as this will affect the amount of energy that can be removed from the core, as well as how much energy is required to circulate the coolant through the core.

All the above points necessitate a thermal hydraulic understanding of the reactor via computational mathematical methods. These models determine
the key variable solution fields (pressure, temperature and velocity) of each present phase via the solution of conservation laws (momentum, energy and mass). The solution of these equations is obtained via a variety of methods but mainly via the deterministic finite volume, finite difference and finite element methods. Each of these methods are closely linked and are variants of weighted residual methods. The finite difference method (FDM) is the oldest based upon a Taylor expansion of the relevant differential equation in strong form. The finite volume method (FVM) is based on conserving physical quantities between discrete volumes of the domain. The finite element method (FEM) divides the domain into sub domains, called elements, and solves for an approximation of the weak form of the relevant differential equation from an expansion of a set of basis functions. The FVM and FEM are more easily applied to complex geometries compared to the FDM and are more commonly used.

When solving for an approximation to an equation with an advection term typically a stabilisation method is required. This is conventionally achieved through standard methods such as Streamline Upwind Petrov Galerkin (SUPG), Control Volume FEM (CVFEM) or Discontinuous Galerkin (DG) methods.

To solve for the momentum and mass balances typically algorithms that iterate between solving for velocity and pressure are used. To further link these balance equations with other field equations such as energy balance further iteration is required.

Typically when solving the flow through a nuclear reactor rather than use a 3D based model a collection of 1D channel models are used with a further model to deduce the inlet boundary conditions. This is acceptable for internal flows but problematic for external flows as it does not fully represent the physics of the problem.

2.4. Coupled Neutron Kinetic Thermal-Hydraulic Modelling

To fully comprehend the complex spacetime dynamics governing a nuclear reactor, a detailed multiphysics analysis is necessary. During the design phase it is desirable to ascertain precise operational limits such that they are not breached during whole lifetime operation. Resulting from the large
scale of the calculation required numerical computational models (codes) are utilised. In the past the multi-physics analysis was performed via breaking the problem down into separate topics (such as neutronic, fluid dynamic and structure mechanics). Calculations were either performed independently of each other or coupled to another using an extremely simplified representation of the secondary topic. These codes provided conservative estimates (hence called Conservative Code) of reactor limits causing the final implied design to perhaps not be the most optimal concerning factors such as safety, reliability and economics. With vastly improved computational power along with continual evolutionary research into numerical algorithms the possibility to perform detailed coupled calculations has become feasible. This method has come to be called the Best Estimate approach Bousbia-Salah and D'Auria (2007), which essentially involves the coupling of two (or more) advanced codes. For an in depth whole core understanding of the reactor dynamics during a transient, it has become generally accepted that the Best Estimate coupled neutronic thermal hydraulic method should be utilised.

During a nuclear reactor transient (such as loss of forced cooling, LOFC) it is vital that the integrity of the core components is not breached, especially the fuel meat and cladding. If the fuel and cladding were to fail then the possibility of unacceptable radiation exposure to the nuclear plant personnel and surrounding environment would greatly increase. In the worst case scenario a large area of populated land could also be contaminated following a full containment breach. Therefore, all nuclear reactor’s should be designed in such a way that a devastating accident has an extremely low probability of occurrence. Also the operating company, institution or government of the reactor should have a detailed knowledge of the operational limits under all postulated accident scenarios. One of the main concerns during a reactor transient is whether certain components such as the fuel, cladding and reactor pressure vessel increase in temperature beyond safe limits. To ascertain the possibility of a reactor design breaching temperature limits requires either an experimental core test or a detailed coupled neutronic thermal hydraulic computational calculation. The latter is more favourable in the design phase and the former would only be attempted intentionally on a proven design for obvious reasons.

As the name suggests, Best Estimate coupled neutronic thermal hydraulic codes involve the solution of the neutron kinetic, fluid dynamic and thermal
transport equations. The solution methods of these individual modules has
been discussed in previous sections. However, although advanced codes and
methodologies exist for the solution of these equations, they are not always
the method implemented into a coupled model. Certainly for the neutronics
module it is still common practice to use a few group neutron diffusion code
rather than a neutron transport code. Currently, coupled neutronic thermal
hydraulic codes are capable of modelling whole cores using 3D geometry with
homogenised fuel assemblies. The out of core components are then modelled
using a 1D representation, or nodalisation. Future research is progressing to
move towards retaining more in-core heterogeneity thus requiring the use of
robust transport codes.

When discussing coupled neutronic thermal hydraulic codes it is important
to distinguish between the various different methodologies that are used in
the coupling process Ivanov (2006), regardless of the solution methods used
in the individual modules. Coupling methodologies can vary in the way the
spatial and temporal inter module coupling is implemented, as well as when
information is exchanged between modules and how the code is written.

The coupling between the in core and out of core modules can either
be internal or external. An external approach would solve for the core
neutronic/thermal-hydraulic and out of core thermal hydraulics separately.
The out of core calculations would provide boundary conditions for the
within core code. An internal approach involves a coupling between a neu-
tronic core model and a whole system (including core) thermal hydraulic
code, where the out of core solution is embedded with the within core solu-
tion. The external approach was first utilised historically due to the ease of
implementation. However the internal approach provides better convergence
and is less susceptible to instabilities occurring, hence is the preferred ap-
proach. This definition of coupling however does provide any insight into the
within core coupling of the neutronic and thermal hydraulic modules. The
coupling here is performed in an iterative manner with the neutronic and
thermal hydraulic modules being called successively until the desired con-
vergence in both is reached. For a transient simulation this internal iteration
would be performed within each time step.

Coupled codes can be also classed as having serial coupling or parallel
processing coupling. In serial coupling the two modules are executed on the
same computer processor. The parallel approach implies each module is ex-
cuted on separate processors and information is exchanged between the two. The parallel approach has the benefit of a shorter simulation time. However, a serial code can also be made to execute on multiple parallel machines via domain decomposition. This would also greatly reduce simulation time. The parallel method is thus greatly favoured.

Coupled codes can also vary in their choice (or available choices) of spatial domain coupling between the two modules. This is represented via a mapping between each modules space. A one-to-one mapping would involve a direct linking between each discrete spatial volume (node or element). Another method involves a different mapping where fuel assemblies with similar neutronic properties and fluxes are mapped to the same thermal hydraulic 1D channel model. This would have to balance the accuracy of the solution with the convergence. This method has become popular for Boiling Water Reactor (BWR) modelling as the individual fuel assemblies are enclosed, so no cross flow exists between fuel assemblies. Where cross flow is prevalent (as in a Pressurised Water Reactor, PWR) the 1D channel approximation is invalid and a full 3D core model is required. Different spatial meshes between this and the neutronic model are also possible options. It is also possible to partition the domain such that certain sub domains have the coupled equations solved and other sub domains have only the neutronic equations solved Pain et al. (2001a), thus reducing the computational resources required. This is particularly useful for normal operational modelling high temperature reactors which have large reflector regions that can be assumed at constant temperature. However, in a transient scenario this would be an invalid approximation as the reflectors provided a temporal heat sink thus requiring a coupled treatment.

Coupling between the time step of each module can easily be achieved by choosing the smallest of the two. If an adaptive time step algorithm is implemented then the smallest of each of these for each module is chosen at each time step.

In common with the general world trend of nuclear reactor preference, Best Estimate coupled neutronic thermal hydraulic codes have been designed and applied to PWR’s and BWR’s. Here the aim was to capture the strong direct feedback between the two modules for improved safety analysis. Recently this has accumulated in benchmark cases where participants analyse various scenarios and compare different codes. One such benchmark proposed was a
Main Steam Line Break (MSLB) in the secondary circuit of a PWR Todorova et al. (2003). This complicated accident would cause a de-pressurisation of the secondary circuit. Under a lower pressure the water would flash boil providing highly efficient heat transfer in the heat exchanger between the primary and secondary circuits. The water circulating in the primary circuit would thus be cooled below normal operating temperatures. When this cooled water returns to the core positive reactivity is induced due to negative temperature coefficient. This would then cause a power excursion in the core. Other benchmark cases have also been carried out for accidents in BWR’s and Russian VVER’s. In all these cases it is crucial to use a 3D model of the whole core to capture any asymmetric dynamics, which could for example result from a control rod ejection. Recently the methodologies and various codes applied to these light water reactors (LWR) have come under review Bousbia-Salah and D’Auria (2007). It is stated that although improved results are obtained using the Best Estimate approach further verification and validation is still required to consolidate methods, due to discrepancies between different codes and from experiments. These discrepancies can be for a number of reasons including approximating material data and the use of empirical equations for constitutive laws. As with all scientific research the human error can often be the largest. A more detailed analysis of coupled codes applied to LWR’s can be found in Bousbia-Salah (2004).

With the recent renewed interest into the HTGR design, due to the possibility of inherent and passive safety as well as improved economics over conventional LWR’s, the Best Estimate coupled approach is gradually been applied to this type of reactor as well. Although a HTGR uses a single phase neutronically inert coolant, implying no direct thermal hydraulic feedback, there is still an indirect feedback from the cooling of core components. There is also the coupling between the neutronics and temperature of the fuel particles due to a strong negative temperature coefficient that provides strong inherent safety. However, there exists only limited published journal research relating to modelling HTGR using the Best Estimate coupled approach, with most of this aimed at the pebble bed design rather than the prismatic block reactor. This reflects the infancy of the approach towards this reactor design with a bias towards building codes aimed at modelling LWR’s. Realising this a recent NEA/OECD benchmark case Reitsma and et al. (2006) has been initiated to verify and validate the few existing
HTGR coupled codes and other LWR coupled codes that are being adapted to model HTGR’s. This benchmark case, as with much HTGR research, is focused on static and transient analysis of the PBMR. Initial results relating to the PBMR268 have shown certain discrepancies between different codes. Even though the same cross section data is used the multiplication eigenvalue differs by 3000pcm between codes. Rather surprisingly no reference Monte Carlo simulation was performed or compared to. There are also slight differences between flux profiles and maximum fuel temperatures (varying from 1042-1079 °C) for a static equilibrium core. An explanation is offered relating to the way the Xenon and Samarium fission product poisoning is incorporated and how certain codes normalise results. This alone illustrates the need to benchmark codes and the reason why regulatory bodies have yet to adopt these more advanced methods. The coupled codes TINTE, VSOP, PANTHERMIX, DALTON-THERMIX, NEM-THERMIX and PARCS-THERMIX have been used in the benchmark analysis. The VSOP code was used in the design of the PBMR, uses a four group finite difference neutron diffusion method in RZ geometry coupled to thermal hydraulic code. Then NEM and PARCS neutron diffusion codes developed at Penn State University and Purdue University respectively were initially coupled to conventional LWR thermal hydraulic codes (such as TRAC and RELAP). The technology and experience is now being applied to HTGR’s with each coupling to the THERMIX code.

The TINTE (TIme dependent Neutronics and Temperature) code Scherer and Gerwin (1990) was developed specifically for HTGR modelling. TINTE solves the two group neutron diffusion and thermal hydraulic equations in RZ geometries using a one dimensional leakage iteration method. Decay heat is incorporated using 14 pseudo decay groups and spatial heat production is split between fission heat produced in the fuel and heat produced from neutron moderation and gamma ray absorption in the graphite. The heterogeneity of the energy transfer from fuel to coolant is accounted for by a sub scale conduction model. TINTE has been compared to actual reactor transient data from the German AVR Scherer et al. (1987). Transients included varying control rod positions and core mass flow rate separately to make an assessment of fuel and moderator reactivity coefficients. However, due to the rapid heat transfer through the fuel element these separate effects could not be distinguished. Instead the overall reactivity coefficient could
only be monitored. Never-the-less, good agreement between TINTE and experiment was observed for the prediction of core power oscillations and final quasi steady state.

The PANTHERMIX (PANTHER-THERMIX) code de Haas et al. (2005) has also been developed specifically for coupled analysis of HTGR, but mainly aimed at the PBMR. PANTHER is a 3D neutron diffusion code using finite difference or nodal techniques. Although it has no RZ cylindrical geometry option it can be approximated with the 3D geometry. The decay heat is calculated using 32 pseudo fission products with stable daughter nuclei. Recently PANTHERMIX has been used in the assessment of burning plutonium in a pebble bed reactor Bende (1999). Normal operation and some coupled transients were performed producing insightful results into the possibility of a plutonium burning PBR.

A recent development has been the CEA research to couple the neutronic code CRONOS2 to the thermal hydraulic code CAST3M and the system code CATHARE for specifically modelling HTGR’s Studer and et.al. (2005). This appears to be produced in a generic way such that general geometries can be used. The reactor physics code APOLLO2 is used to generate the collapsed group constants. Each module has and continues to be validated against experiments and international benchmarks. Some initial static results for steady state coupled calculations for a block type VHTR using a \( \frac{1}{6} \) whole core model have been performed. Triangular prism meshes are used within each module with a mapping between them such that different mesh resolutions can be used. The ability to use a non-conforming mesh allows explicit modelling of control rod channels in the whole core model. The initial results mainly focused on finding the minimum required number of elements for each module in the axial and radial direction. The optimal model is found to require around 85000 elements for the \( \frac{1}{6} \) whole core model. No transient results are given or known yet. More steady state results for this coupled code called NEPHTIS are given in Limaiem et al. (2006). A discussion of how the double heterogeneity is accounted for, via a submodel, in the energy transfer through the solid is briefly given. As the model is steady state this submodel is calculated analytically. The core Keff evolution with burnup is shown with and without reflector control rods. Power is shown to peak in the upper region of the active core and temperature in the lower. The fuel and moderator temperature reactivity coefficient are shown
to be negative for the full burnup cycle, with the fuel the larger of the two. Peak fuel temperatures are found to be around 1200°C at steady state.

The coupled neutronic CFD code FETCH used for this research is presented in detail in the next section.

2.5. The Methodology of FETCH

2.5.1. Introduction

FETCH (Finite Element Transient Criticality) Pain et al. (2001a) is a coupled deterministic radiation transport multiphase fluid dynamic code implemented within the finite element framework. The finite element method (FEM) Zienkiewicz et al. (2005) has great geometrical flexibility allowing the possibility of complex domains (such as nuclear reactor cores) to be modelled in similar detail compared with stochastic Monte Carlo methods (with enough computational resources) in certain instances. FETCH consists of four modules; the preprocessor GEM, a neutronic module, a multiphase fluids module and an interface module.

The neutronics module (called Even Parity Neutral Particle Transport, EVENT) de Oliveira (1986) solves the Neutron Boltzmann Transport equation in full phase space based on a second order even-parity variational finite element formulation, using spherical harmonics to discretise the angular dependence of the neutron flux (or photon flux). The energy dependence is modelled via the common multi-group method forming a set of discrete energy transport equations that are coupled through the intergroup (up-scatter as well as down scatter) scattering source terms. The neutronics module can be applied to transient simulations (with non-linear feedback from the fluids module) and also to static simulations to obtain the multiplication factor (k-effective) for the input domain.

The multiphase fluid dynamic module (FLUIDITY) Piggot (2009) Gomes (2004) solves the non-linear momentum transport and continuity equations, as well as advection-diffusion equations for any other variable fields as desired (e.g. temperature). FLUIDITY uses a variety of discretisation methods such as standard Galerkin, Petrov-Galerkin and has the capability to perform Large Eddy Simulation (LES). The coupling between each phase is through the use of relevant empirical heat and momentum transfer correlations that
are dependent on the physical problem being simulated. Within each of the neutronic and fluid dynamic modules a choice of finite elements is available, as well as the ability to simulate in Cartesian or cylindrical coordinates. Implemented adaptive time stepping ensures the relevant physics is captured while maximising computational simulation speed.

The interface module passes updated information like temperature fields and sources (due to fission) between the other two modules within each time step. The neutronics module uses the updated fields (which can include changes in material composition) to interpolate for new cross sections within each finite element. The fission source generated in the neutronic module produces a heat source for the fluids module introducing a feedback into the simulation. The cross sections are interpolated between a pre-determined data set generated using the reactor physics WIMS9 code of Serco Assurance ANSWERS-WIMS. The WIMS9 code generates macroscopic group cross sections using a variety of techniques such as collision probability methods, then collapses them to the desired number of energy groups (usually 6 groups). A characteristic geometry is used within the WIMS9 input file and resonance self-shielding effects are accounted for, as well as temperature and density changes, in the generation of group constants. Within FETCH the cross sections are taken as piece-wise constant over each element of the domain and interpolated between linearly.

Each module reduces the relevant partial differential equations to a set of simultaneous linear equations, the number of which depends on the number of finite elements and the order of the basis function approximation used. These are then solved for using various iterative techniques such as the pre-conditioned conjugate gradient method and the generalised minimum residual method (GMRES).

The coupled FETCH code has been applied to the modelling of criticality accidents in fissile solutions Pain et al. (2001b). Results were validated against actual experimental data and compared to other criticality codes. Due to showing good agreement with available data, FETCH has also been applied to scenarios where there exists limited experimental knowledge. This includes modelling criticality in plutonium solutions Pain et al. (2001c) and a novel fluidized HTGR Pain et al. (2003) Pain et al. (2005). FETCH is now being applied to a variety of nuclear reactors. The radiation transport module EVENT has also been validated for various benchmark simulations.
Ziver et al. (2005) de Oliveira et al. (2001) Keller and de Oliveira (2004) and applied to a variety of scenarios such as nuclear reactors, atmospheric clouds and nuclear well-logging. The CFD module FLUIDITY has been applied to model fluidised beds, oceans, atmospheric pollution and more recently asteroid crater impacts.

In the following sections a more in-depth description of the methodology behind each module of the FETCH model is described, outlining the underlying mathematical equations.

2.5.2. The Neutronic Module

In this section the Boltzmann Transport Equation is described and the formulation to the second order even parity form outlined. The numerical method used within FETCH for solving the resulting equation is then illustrated.

2.5.2.1. The Neutron Transport Equation

The simulation of neutral particles through a domain has many applications including the transport of photons through clouds, nuclear well-logging and nuclear reactors. In the latter the description of the neutron density is crucial to understanding the complex reactions occurring across a complicated domain. The transport of neutral particles is mathematically described via the linear neutral particle Boltzmann Transport equation Lewis and Miller (1993), an adaptation of the Boltzmann Transport equation formulated for gases. The Neutron Transport equation describes the evolution of a neutral particle density field in full phase space (Cartesian space, angle, energy, time), which is derived using a continuum assumption. Although in reality the particles are discrete, the continuum assumption will hold provided the space-time discretisation used is large compared with the underlying space-time scales associated with individual nuclear reactions (typically less than $O(10^{-10})$ which is well beyond the limit of any present and future computation). Using this assumption and considering the various source and sinks influencing the particle density, the neutral particle Boltzmann Transport equation describing the angular flux density across a domain is given by:

$$\frac{1}{v} \frac{\partial \psi(r, \Omega, E, t)}{\partial t} + \Omega \cdot \nabla \psi(r, \Omega, E, t) + \mathcal{H} \psi(r, \Omega, E, t) = S(r, \Omega, E, t) \quad (2.4)$$
where \( S(r, \Omega, E, t) \) is the source term and \( \mathcal{H} \) is the scattering removal operator given by

\[
\mathcal{H} \psi(r, \Omega, E, t) = \Sigma_f(r, E, t) \psi(r, \Omega, E, t) - \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_s(r; E' \rightarrow E; \Omega' \rightarrow \Omega; t) \psi(r, \Omega, E, t).
\]  

The variable \( \psi(r, \Omega, E, t) \) represents the angular flux density at each point, denoted by \( p \), in the phase space (i.e. at position \( r \), in direction \( \Omega \), with energy \( E \) and at time \( t \)). If the scattering is assumed to be independent of the incident angle, such that only the change in angle matters, the scattering removal operator can be written explicitly by

\[
\mathcal{H} \psi(r, \Omega, E, t) = \sum_{l=0}^{\infty} \frac{2l + 1}{4\pi} \int_0^\infty dE' (\Sigma_f - \Sigma_{sl}(r; E' \rightarrow E, t)) \int_{4\pi} d\Omega' P_l(\Omega \cdot \Omega') \psi(r, \Omega, E, t),
\]  

where \( P_l \) are the Legendre Polynomials and \( \Sigma_{sl} \) are the scattering moments. The angular flux is related to the angular density, \( N(r, \Omega, E, t) \), via

\[
\psi(r, \Omega, E, t) = v N(r, \Omega, E, t),
\]  

where \( v \) is the speed of the neutral particles. By considering a small control volume \( dp \) in the phase space given by

\[
dp = dV d\Omega dE,
\]  

where \( dV \) is a control volume in real space \( \mathbb{R}^3 \), then \( \psi(r, \Omega, E, t) dp \) represents the angular flux density in \( dV \) about \( r \), with direction \( d\Omega \) about \( \Omega \) and energy \( dE \) about \( E \) occurring at time \( t \).

The first term on the left of equation (2.4) represents the rate of change of the angular flux density at every point within the phase space. The second term on the left given by \( \Omega. \nabla \psi(r, \Omega, E, t) \), called the streaming term, represents the net rate at which the angular flux density advects away from every point in the phase space. The scattering removal operator, \( \mathcal{H} \), represents the rate at which the angular flux density is removed from phase point \( p \) via absorption with the host medium present in the domain, minus the rate at
which the the angular flux density is scattered from phase point \( p' \) to phase point \( p \), due to interactions again with the host medium. Note that \( p' \) could be a phase point with a different energy or a different direction or both. The term \( \Sigma_t(r, E, t) \) is the total (scattering and absorption) macroscopic cross section, with units \( cm^{-1} \), between the host medium and the angular flux density at phase point \( p \). The term \( \Sigma_s(r; E' \rightarrow E; \Omega' \rightarrow \Omega; t) \) is the double differential macroscopic scattering cross section representing the probability that the angular flux density with energy \( E' \) and direction \( \Omega' \) will scatter with the host medium into energy \( dE \) about \( E \) and direction \( d\Omega \) about \( \Omega \), for all points in the phase space. Note that the time dependence of the macroscopic cross sections arises due to their dependence on the number density of the host medium, which may change with time. The source term \( S(r, \Omega, E, t) \) represents all sources of neutral particles including external. In deriving equation (2.4) there are some implicit assumptions made. These include assuming point particles, instantaneous reactions, external forces don’t affect the motion of the neutral particles and no particle particle reactions occur. The latter assumption is valid provided the number density of the host medium is far greater than the number density of the neutral particles, which is often the case.

For neutrons within a nuclear reactor the source term is given by

\[
S(r, \Omega, E, t) = S_{\text{ext}} + \left( 1 - \beta_{\text{eff}} \right) \chi_p \int_0^\infty dE' \int_{4\pi} d\Omega' \nu(E') \Sigma_f(r, E', t) \psi(r, \Omega', E', t) + \sum_k \lambda_k \chi^d_k C_k(r, t),
\]

(2.9)

where the first term on the right represents external neutron sources and the other two terms are the prompt and delayed fission neutrons respectively. In this relation \( \beta_{\text{eff}} \) represents the fraction of neutrons that are delayed, \( \chi_p \) is the prompt fission spectrum, \( \chi^d_p \) is the delayed fission spectrum from delayed precursor group \( k \), \( C_k \) is the delayed neutron precursor concentration for delayed group \( k \), \( \lambda_k \) is the decay constant for delayed group \( k \), \( \nu \) is the number of neutrons emitted per fission event and \( \Sigma_f(r, E', t) \) is the macroscopic fission cross section. The delayed neutron precursor groups represent the fission products that beta decay to a daughter that spontaneously decays via neutron emission, with characteristic decay constants and fission yields.
for each group. The delayed neutrons created in these processes are vital for control of the nuclear reaction. The governing equation for the $k^{th}$ delayed neutron precursor group is given by

$$\frac{\partial C_k(r, t)}{\partial t} + u \cdot \nabla C_k = -\lambda_k C_k(r, t) + \beta_k \int_0^\infty \nu(E') \Sigma f(r, E', t) \phi(r, E', t),$$

(2.10)

where $u$ is the velocity of the host medium (if any), $\beta_d$ is the fraction of delayed neutron precursor group $k$ produced via fission and $\phi(r, E', t)$ is the scalar flux given by

$$\phi(r, E', t) = \int_{4\pi} \psi(r, \Omega', E', t) d\Omega'.$$

(2.11)

The Neutron Transport Equation (2.4) is a first order hyperbolic integro-differential equation that can in theory provide an exact description of the time dependent neutron distribution, provided the assumptions of the derivation are based on hold for the particular problem in question. In practice an exact analytical transport solution is only possible for certain idealised problems which are based on further assumptions. Equation (2.4) is extremely hard to solve for realistic problems due to the angular flux depending on seven variables $(x, y, z, \theta, \phi, E, t)$ and due to the complex dependence of the macroscopic cross sections on position and energy. The numerical solution can be obtained by discretising each variable of the angular flux using a variety of schemes. These could be applied directly to the first order neutron transport equation (2.4) or to alternative variations of it, such as the second order even parity neutron transport equation. As with all differential equations to obtain a particular solution, boundary and initial conditions are necessary. For the initial condition $\psi(r, \Omega, E, t) = \psi_0(r, \Omega, E, t)$ two common boundary conditions are

$$\psi(r, \Omega, E, t) = 0 \quad \text{for } r \in \Gamma_V, n \cdot r < 0,$$

(2.12)

$$\psi(r, \Omega', E, t) = \psi(r, \Omega, E, t) \quad \text{for } r \in \Gamma_V$$

(2.13)

where $\Gamma_V$ is on the boundary to the domain $V$, $n$ is an outward point normal vector to this boundary and $\Omega'$ is the reflected angle corresponding to the incident angle $\Omega$. The first condition is the vacuum boundary condition and the second is the reflect boundary condition. The second boundary condition
can be generalised to become a surface source condition, where this source is the angular flux in the reflected direction for the reflect boundary condition.

In the next section the second order even parity neutron transport equation will be formulated and the solution method implemented within FETCH will be illustrated.

2.5.2.2. The Second Order Even Parity Neutron Transport Equation

In the previous section the first order neutron transport equation was introduced. In this section the formulation to the equivalent even and odd parity neutron transport equations are outlined, then the second order even parity neutron transport equation is formed. The benefits of this approach and the discretisation methods used within FETCH are also stated.

The first step is to separate the angular flux into even and odd parts via the Vladimirov transformation given by

\[
\psi_{\text{even}}(r, \Omega, E, t) = \frac{1}{2}(\psi(r, \Omega, E, t) + \psi(r, -\Omega, E, t)) \quad (2.14)
\]
\[
\psi_{\text{odd}}(r, \Omega, E, t) = \frac{1}{2}(\psi(r, \Omega, E, t) - \psi(r, -\Omega, E, t)) , \quad (2.15)
\]

where

\[
\psi(r, \Omega, E, t) = \psi_{\text{even}}(r, \Omega, E, t) + \psi_{\text{odd}}(r, \Omega, E, t). \quad (2.16)
\]

By substitution of \(\Omega \rightarrow -\Omega\) into (2.4) it can be seen that

\[
\frac{1}{v} \frac{\partial \psi(r, -\Omega, E, t)}{\partial t} - \Omega \cdot \nabla \psi(r, -\Omega, E, t) + \mathcal{H} \psi(r, -\Omega, E, t) = S(r, -\Omega, E, t), \quad (2.17)
\]

where it is recognised that a negative will appear in the double differential scattering cross section relating to the angle difference variable. It can be shown that by adding equation (2.4) to (2.17) and by subtracting equation (2.17) from (2.4) gives the coupled even-odd parity neutron transport
equations:

\[
\begin{align*}
\frac{1}{v} \frac{\partial \psi^{\text{even}}}{\partial t} + \Omega \cdot \nabla \psi^{\text{odd}} + C \psi^{\text{even}} &= S^{\text{even}} \quad (2.18) \\
\frac{1}{v} \frac{\partial \psi^{\text{odd}}}{\partial t} + \Omega \cdot \nabla \psi^{\text{even}} + G^{-1} \psi^{\text{odd}} &= S^{\text{odd}}, \quad (2.19)
\end{align*}
\]

where the source has been transformed into even and odd parity components and the operators \( C \) and \( G^{-1} \) are given by:

\[
\begin{align*}
C \psi^{\text{even}} &= \Sigma_t(r, E, t) \psi^{\text{even}} \\
&\quad - \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_{s}^{\text{even}}(r; E' \to E; \Omega' \to \Omega; t) \psi^{\text{even}} \\
G^{-1} \psi^{\text{odd}} &= \Sigma_t(r, E, t) \psi^{\text{odd}} \\
&\quad - \int_0^\infty dE' \int_{4\pi} d\Omega' \Sigma_{s}^{\text{odd}}(r; E' \to E; \Omega' \to \Omega; t) \psi^{\text{odd}}, \quad (2.21)
\end{align*}
\]

where the macroscopic scattering cross section has also been decomposed into even and odd parity components. By a simple substitution for the odd parity angular flux, the steady state second order transport equation for the even parity angular flux is given by:

\[
\begin{align*}
-\Omega \cdot \nabla (G \Omega \cdot \nabla \psi^{\text{even}}(r, \Omega, E, t)) + C \psi^{\text{even}}(r, \Omega, E, t) \\
= S^{\text{even}}(r, \Omega, E, t) - \Omega \cdot \nabla G S^{\text{odd}}(r, \Omega, E, t). \quad (2.22)
\end{align*}
\]

At each time step of a transient simulation FETCH solves equation (2.22) with modified terms to include the solution from the previous time step. For a steady state calculation to obtain the multiplication factor FETCH solves equation (2.22) with a modified source term to include the criticality eigenvalue, via a power iteration method. By solving for the even parity angular flux the odd parity angular flux can be ascertained. The even and odd angular flux components have physical significance which can be seen by integrating them over all directions such that:

\[
\begin{align*}
\phi(r, E, t) &= \int_{4\pi} \psi(r, \Omega, E, t) = \int_{4\pi} \psi^{\text{even}}(r, \Omega, E, t) \quad (2.23) \\
J(r, E, t) &= \int_{4\pi} \Omega \cdot \psi(r, \Omega, E, t) = \int_{4\pi} \Omega \cdot \psi^{\text{odd}}(r, \Omega, E, t), \quad (2.24)
\end{align*}
\]

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where \( \phi(r, E, t) \) is the scalar flux and \( J(r, E, t) \) is the neutron current which represents the net rate at which neutrons pass through a unit surface area. To obtain a solution to equation (2.22) a variational procedure is used in that it is recognised that an equivalent problem involves finding the function that minimises the functional

\[
F[\psi] = \langle \Omega \cdot \nabla \psi, G \Omega \cdot \nabla \psi \rangle + \langle \psi, C \psi \rangle - 2\langle \psi S^{even} \rangle - 2\langle \Omega \cdot \nabla \psi, G S^{odd} \rangle,
\]  

(2.25)

with respect to small variations (where \( \langle v, u \rangle \) is short hand for the inner product of \( u \) and \( v \)). The Functional must be chosen such that when minimised equation (2.22) is obtained as a Euler-Lagrange equation. In seeking to minimise equation (2.25) the domain is partitioned into a set of non-overlapping sub domains, called elements. Within each element the solution \( \psi \) is approximated by a trial function, \( \psi^\delta \) given by the expansion

\[
\psi^\delta = \sum_{j=1}^{N} \sum_{k=1}^{M} B_j(r) Q_k(\Omega) \Psi_{jk},
\]  

(2.26)

where \( B_j(r) \) are the spatial basis functions (usually piece-wise linear), \( Q_k(\Omega) \) are the angular basis functions and \( \Psi_{jk} \) is the moment coefficient matrix of unknowns. Within FETCH the angular basis functions are given by the normalised spherical harmonic functions. Using this trial function in minimising equation (2.25) a set of linear equations is obtained where the unknown coefficient matrix is sort. Due to the formulation this matrix has certain useful properties such as being sparse (due to the compact nature of the basis functions) and being symmetric positive definite, which allows efficient numerical algorithms like the preconditioned gradient method to be used. The advantages of using spherical harmonic basis functions include the absence of ray effects often found in discrete ordinate methods. Within FETCH there is no restriction on the order of approximation concerning the spherical harmonics expansion. The energy variable is discretised using a multigroup method producing a set of coupled transport equations that are linked through their source terms due to inter-group scattering (upscat as well as downscatter).

In the next section the solution of the fluid dynamic equations imple-
mented within FETCH is outlined.

2.5.3. The Multiphase Fluid Dynamic Module

The fluid dynamic module is a general purpose CFD package (FLUIDITY) that solves the non-linear momentum equations, continuity equation and any desired general variable advection-diffusion equation. The discretisation methods include the stabilisation Petrov Galerkin technique. FLUIDITY also has the capability to solve the multiphase fluid dynamic equations linking each phase through relations for momentum and energy transfer, which are often obtained empirically. The Navier Stokes equations which are numerically solved for in FETCH, that govern the conservation of momentum and mass for two fluid flow, are given by:

\[
\frac{\partial}{\partial t} (\epsilon_k \rho_k v_k^i) + \frac{\partial}{\partial x_j} (\epsilon_k \rho_k v_k^j v_k^i) = -\epsilon_k \frac{\partial p}{\partial x_i} + \epsilon_k \rho_k g_i + \beta (v_{k,\text{other}}^i - v_k^i) + \frac{\partial \tau_{kij}}{\partial x_i}
\]

(2.27)

and

\[
\frac{\partial}{\partial t} (\epsilon_k \rho_k) + \frac{\partial}{\partial x_i} (\epsilon_k \rho_k v_k^i) = 0,
\]

(2.28)

where \( k \) represents a phase, \( \epsilon_k \) is the volume fraction (porosity) for phase \( k \), \( v_k^i \) is the velocity for phase \( k \) (unless stated otherwise) in the direction \( i \), \( \rho_k \) is the density for phase \( k \), \( \tau_{kij} \) is the stress tensor for phase \( k \), \( p \) is the pressure, \( g_i \) is the gravitational force in direction \( i \) and \( \beta \) is the momentum exchange coefficient between the two phases. The thermal energy equation associated with each phase is given by

\[
\epsilon_k c_p \rho_k \left( \frac{\partial T_k}{\partial t} + \frac{\partial}{\partial x_i} (T_k v_k^i) \right) = \frac{\partial}{\partial x_i} \left( \epsilon_k k_k \frac{\partial}{\partial x_i} T_k \right) + \alpha (T_{k,\text{other}} - T_k) + Q_k,
\]

(2.29)

where \( T_k \) is the temperature of phase \( k \), \( c_p^k \) is the specific heat capacity of phase \( k \), \( k_k \) is the conductivity of phase \( k \), \( \alpha \) is the volumetric averaged heat transfer coefficient and \( Q_k \) is a volume source term that could include energy from internal fluid friction. Within FETCH the energy source term due to
the nuclear fission is given by

$$Q^k(r, t) = \int_0^\infty dE \omega \Sigma^k_f(r, E, t) \phi(r, E, t),$$

where $\phi$ is the scalar flux field, $\Sigma^k_f$ is the fission macroscopic cross section and $\omega$ is the energy released per fission event (around 200MeV for $U^{235}$).

Note that it is assumed that all the energy is released instantaneously and all at the point of where fission occurs. The boundary conditions can consist of a range of possibilities, such as Dirichlet, Neumann and Robin conditions.

The fundamental equations are discretised by first constructing a mesh for the entire domain. Within each element of the mesh the fluid field variables are approximated via an expansion of a set of basis functions. Continuous linear Lagrange functions for the velocity field and piecewise constant functions for the pressure field are used (the pressure field must be expanded with basis functions of order less than the velocity to avoid a singular matrix problem). By discretising the time derivative using a standard theta method the discretised momentum equation becomes

$$A \frac{u^{n+1}}{\Delta t} = C p^{n+1} + B^{n+1} + S^n.$$  

The superscript denotes the time level at which the associated variables are evaluated. The $A$ matrix contains the implicit coupling between the phases as well as the implicit discretisation of the momentum advection and diffusion terms within each phase. The $C$ matrix is associated with the pressure gradient force, the $B$ vector contains the gravity body force and the $S$ vector contains the driving contribution from the previous time step. This discretised force balance combined with the discretised continuity equation and an equation of state are used to solve for the velocity, pressure and density iteratively Pain et al. (2001d). A projection method combined with correction factors for the velocity and pressure is used. A non linear Petrov Galerkin method is used to stabilise the momentum equations Hughes and Mallet (1986). The energy balance equations of each phase are discretised using a Control Volume Finite Element Method (CVFEM) AMCG (2010). A Picard iteration is used to couple the different phases energy, momentum and continuity equations together. A fully implicit backward Euler time stepping scheme to maintain stability is used for all solution variables.
An adaptive time stepping algorithm that considers the rate of change of the solution variables as well as the number of Pickard iterations is used to maximise computational efficiency. The matrix equations are solved using iterative techniques such as the Generalised Minimum Residual Method (GMRES) to a prescribed accuracy.

In the next section the calculation method within FETCH is illustrated.

2.5.4. The Flow Structure of FETCH

In this section the flow structure of FETCH will be illustrated to show how non-linear feedback mechanisms can be captured, an essential condition for modelling nuclear reactor transients. Initially a set of macroscopic group cross sections are generated using the code WIMS9 for the desired range of temperature and burnup for each material. Then within each adaptive time step the following iterative algorithm occurs until the specified convergence is met.

1. Using the beginning of time step temperature and material distribution, a cross section is obtained for each element in the mesh via interpolating the predetermined different temperature and burnup cross sections.

2. The Neutron Transport equation is then solved for each energy group to obtain the angular flux for the entire domain.

3. The delayed neutron precursor concentration equations are then solved for each group (usually six) using the scalar flux for calculating the source term.

4. The temperature equations (one for each phase if multiphase) are then solved with the scalar flux providing the fission heat source.

5. Finally the Navier Stokes equations (momentum and continuity for each phase) are solved subject to given boundary and initial conditions, with the temperature field providing a buoyancy force in the fluid phase.

This allows temperature, density and material changes to be captured in determining the neutron distribution across the domain, which is the fundamental requirement needed for nuclear reactor modelling. During a transient
simulation this non linear feedback (characterised by reactivity coefficients) will allow a detailed determination of the coupled multi-physics processes that occur in reality, accurately describing the sequence of events that will unfold in a Best Estimate approach.
Chapter 3

FETCH AUTOMATED VERIFICATION AND VALIDATION

Synopsis

Verification and validation are a necessary process of computational mathematical modelling to provide credibility to any assertions that stem from the model solution. Verification quantifies computational and mathematical model correctness whereas validation quantifies physical model accuracy. They provide evidence to support theoretical explanations and hypothetical predictions. Without evidence any model assertion is baseless. As computational mathematical models are in a continuous state of evolution so must the verification and validation process to maintain credibility and reliability. This chapter presents the application of an automated framework for the continuous verification and validation of the coupled radiation transport fluid dynamic FETCH model. This framework is a recent innovation within the Applied Modelling and Computation Group (AMCG) at Imperial College and is flexible to the extent of being applicable to any computational model. A range of examples that are part of the continuous automated FETCH test case suite are presented including time dependent examples. The development of new multigroup diffusion solver that resulted from this process is also described.
3.1. Introduction

Mathematical modelling is a complementary scientific process with experimental and observational investigation to understand characteristics of reality for a particular purpose. Mathematical modelling is the process of constructing and using a simplified representation of a subset of reality to assert a meaningful explanation or prediction of a quantity of significant interest in a usable form. The assertion is considered meaningful and usable if there is perceived to be sufficient evidence to justify it. Validation aims to quantify the degree of physical accuracy of a model via direct comparison with observation or controlled experiment. Validation thus resides in the realm of the scientific area of interest, such as physics, chemistry, biology, geology.

Mathematical modelling has evolved to a level of complexity such that computational implementation is a necessity. Computational models do not think but perform the instructions inscribed within them by a human. Humans are in general fallible. This implies that the implemented computational instructions of a model may not be as originally intended. Verification aims to reduce the occurrence of imperfections in model implementation with respect to the proposed initial specification, thus quantifying the degree of correctness of a model. Verification also involves quantifying the degree of
mathematical accuracy of a models solution to the exact solution of the mathematical model, irrespective of any physical significance. Verification thus resides in the realms of mathematics and usually computational science.

Therefore verification and validation (V&V) are necessary procedures in deducing the correctness and accuracy of a model so as to provide credibility. Without this credibility the model is effectively useless and thus unable to provide any physically meaningful information. Computationally implemented mathematical models are often in a continuous state of evolution. This not only refers to the associated direct software but also to any related auxiliary software and the hardware architectures available. Thus for a model to retain correctness and accuracy the V&V process must also be in a continuous state of evolution to maintain credibility and importantly reliability.

The primary purpose of this chapter is to assert reliability in the FETCH code to be used as a predictive tool in the proceeding chapters. This chapter is organised as followed. Initially an overview of V&V in general is given. V&V conducted on the FETCH code not directly a part of this research is then presented. A description, including highlighting the benefits, of the automated V&V framework developed within AMCG follows. The current test case suite developed as part of this research is then outlined. A selection of test cases including time dependent are then analysed more rigorously. The development of new multigroup diffusion solver that resulted from this process is also described. Finally conclusions are stated with respect to what was achieved and what is considered a future necessity.

3.2. Verification and Validation

This section gives an overview of V&V procedures. It is by no means a rigorous or complete description. The definitions and descriptions of this section are summaries of those found in the open literature Oberkampf and Trucano (2008), Oberkampf and Trucano (2002), Grace and Taghipour (2004), Babuska and Oden (2004), Szabo and Actis (2009), Greenwald (2010), Kleijn (2003) and the Imperial College reports Farrel et al. (2009), Pain et al. (2008a), Pain et al. (2008b). The literature referenced (and their references) cover a range of physical science disciplines and have prominently appeared within the past decade. Many describe in detail definitions, best practices
and future directions with regard to V&V procedures. Differences in terminology and of what constitutes acceptable V&V is highlighted between different disciplines in the past. The reviews clearly show however that convergence of V&V standards is occurring but significant progress is still required. Emphasis for future directions focuses on community shared rigorously defined verification benchmarks and experiments designed specifically for the purpose of validation.

Also an important point that is frequently asserted is that full verification and validation is simply not viable and probably impossible. Sufficient evidence can be accumulated to assert a subjective degree of confidence with regard to correct model implementation and expected solution errors. Also sufficient (being open to interpretation) evidence can be accumulated to assert that the model is physically valid within a certain range of accuracy to a limited range of scenarios, bearing in consideration the observational or experimental error inherent within this conclusion. Any application of a mathematical model beyond the validity domain (or points) should be considered a hypothetical prediction that can only be justified through interpolation or extrapolation between the (considered) known validity points. This follows the widely regarded philosophical argument inherent to modern scientific thought that theories can never be proved but can only be unproven. As mathematical models derive from scientific theories the argument recursively filters through.

Another important point is what exactly constitutes acceptable tolerances of correctness, error and accuracy of a model. Specification of tolerances is effectively arbitrary and highly subjective. Nevertheless, the tolerances of model correctness and error (verification) should effectively be set to as that capable within machine/computer precision for the fully converged discretization. Tolerances for validation are much harder to specify. This often leads to vague generalisations in conclusions drawn from validation exercises such as "good, fair, poor". Without a clear definition of these terms nothing is gained in the conclusion by using such descriptions. A desired tolerance should initially be stated beforehand with a reason for choosing.

A complication to model validation is model calibration. Model calibration involves adjusting, or fine tuning, one or more input parameters such as to achieve improved comparison of system responses of interest with that of experiment or observation. While this may improve the model system re-
sponses that are compared it does not necessarily improve any other system responses that are not compared. Also model calibration does not necessarily improve model validation as it may be possible to perform different adjustments to achieve the same outcome. The necessity for adjustments indicates model theory (including assumptions) flaws that should be revisited.

It is generally considered obvious that the verification process should precede the validation process. Also the verification process should always be possible to perform. Validation is substantially more difficult due to the requirement of sufficient reliable experimental and/or observational data. This requires more work, skills, knowledge, often people and resources. In certain applications whole model validation may not be possible and must be justified from extrapolation of simpler scenarios and/or through a process of individual components of models validation. Indirect validation of a particular code that embodies a particular mathematical model could also be inferred from the validation process applied to that of a similar code that embodies the same (or considered close enough) mathematical model, assuming sufficient verification.

It is also generally considered important to have an independent V&V process performed. The reason being to remove bias (either positive or negative) from conclusions on model suitability. This however is not always possible and should be considered when reviewing conclusions for impartial fairness.

The most commonly quoted definitions of V&V that occurred within the literature are:

1. Verification: The process of determining that a model implementation accurately represents the developer’s conceptual description of the model and the solution to the model.

2. Validation: The process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended uses of the model.

These definitions are taken directly from Oberkampf and Trucano (2008) where it is also stated that a significant number of scientific and engineering institutions within the U.S.A. have adopted them. Verification consists of
Figure 3.1.: Outline of code verification Oberkampf and Trucano (2008).

code verification and solution verification. Code verification aims to show the correctness of the computational implementation whereas solution verification aims to show the correctness of the model solution to solve the mathematical problem. Solution verification should provide an estimate of the error and convergence of the discrete models solution to assert the applicability of the method inherent within the model to solve the model equations. Code verification can be further divided into numerical algorithm verification and Software Quality Engineering (SQE) practices as illustrated in figure 3.1.

Numerical algorithm verification aims to provide evidence of the mathematically correct implementation of the numerical algorithm. SQE aims to provide evidence of a reliable and correctly implemented code from a practical programming perspective. A code could hypothetically have no implementation errors associated with SQE but have errors associated with the numerical algorithm implementation. Any SQE error will have an effect on deducing the mathematical correctness of the algorithm although SQE errors could go unnoticed if not explicitly tested for. SQE provides evidence of computational programming correctness. SQE practices involve
best practice programming (for example modular), literally checking code (which could include independent checks), unit tests, using different compilers and the use of common debugging tools such as GDB and Valgrind. Regression tests are also a SQE process in that they check the repeatability of the code structure although can not assert anything more.

Numerical algorithm verification involves comparing the model output to that of highly accurate reliable solution. Closed form analytic solutions and Method of Manufactured Solutions (MMS) Roache (2002) Salari and Knupp (2000) are considered the most accurate and reliable for comparison. Closed form analytic solutions are usually only known for what are considered numerically simplistic problems. MMS are however capable of being of general complexity. Non closed form analytic solutions and high confidence numerical solutions are justifiably benchmarks, provided these themselves are verified. The latter includes code to code comparisons where different codes may be using different algorithms to solve the same mathematical equations of the model. Code to code comparisons are also satisfactory for solution verification if each code is implementing the same numerical algorithm and satisfactory evidence is available with respect to code verification. Individual components of the numerical algorithm could also effectively be tested separately as unit tests.

A point not always highlighted is that an error is also potentially inherent within the input data associated with the model. For example this could include geometry, materials and options. Input error can be reduced via repeatedly checking data, obtaining an independent check and analysing output data for anomalies. The larger the amount of user generated directly input data, such as via a keyboard, the greater the possibility of error. Thus input error probability can be reduced through more automated input, with the code performing this task itself requiring verification. This important issue is discussed as certain models can have more lines of data input than lines of code. Input error is due to user error. Therefore even if substantial evidence is accumulated through a V&V process, every application and conclusion asserted from the generated solution is always susceptible to user error. User error can be reduced through rigorous Quality Assurance (QA) procedures. QA includes V&V as well as peer review, efficient management, maintenance, documentation and social interaction between users and developers which could include training.
Even though verification can be decomposed into solution verification, SQE and numerical algorithm verification, the actual process of acquiring evidence for each may be indistinguishable. This is because each may be tested through running the code on the same problem. Also if this test case has a physical significance with a reference experimental answer then the process can also become a validation as well, provided the required verification is obtained.

Validation procedures are not discussed herein. Detailed descriptions of suggested procedures to construct and perform validation exercises are given in the referenced literature such as Oberkampf and Trucano (2008) and Pain et al. (2008b). It is recognised that rigorous validation of a large multipurpose multiphysics model such as FETCH is extremely difficult.

A final point is that it is common in radiation transport research to compare deterministic models (such as Finite Element based methods) to stochastic models (such as Monte Carlo based methods). The deterministic and stochastic models are different although are derived from the same physical science. The assertion of different assumptions produces different mathematical models. However, they are capable of being compared as the same type of model system response data can be obtained. From the definitions given above this type of comparison is classified as verification (numerical algorithm and solution) where the stochastic solution is considered as an highly accurate reference. This of course assumes that the stochastic code has evidence to support its own verification claims.

3.3. Overview Verification and Validation
conducted on the FETCH code

This section gives an overview of V&V conducted on the FETCH code that was not directly part of this research. It is a summary of the Imperial College internal reviews Pain et al. (2008a) and Pain et al. (2008b). The FETCH code currently consists of the following components:

1. GEM the FEM preprocessor.
2. EVENT the Radiation Transport solver.
3. FLUIDITY the Computational Multiphase Fluid Dynamic solver.
4. EVENT-FLUIDITY interface.

5. Output analysis tools such as PLOTTER and PARAVIEW and other smaller auxiliary scripts.

Each of these components need to be considered for the V&V process. The individual components of the FETCH code have been under development for twenty years at Queen Mary College and Imperial College London. The primary focus of the code development was for academic research rather than for the industrial/commercial market. Quality Assurance activities are therefore not expected to be as rigorous as that within an industrial setting, although this point is arguable and case dependent. This is not a reflection of the capabilities of the developers and users but more a consequence of the economic support available being limited.

Only verification need be considered for the last component listed. This is usually done implicitly by the developer and the expert user community. Code to code comparison is usually sufficient to deduce correctness of the output analysis tools. Also it is usually common to be utilising more than one output analysis tool such that any inconsistencies should be apparent. Output analysis tools do not directly affect the FETCH results but process FETCH results into a more appropriate form. This processing requires reliable code verification with most emphasis on SQE practices. Output analysis tools, such as PARAVIEW and MAYAVI, used for FETCH result visualisation are open source community driven projects. This implies a community driven continuous verification process and are considered reliable tools.

The FEM preprocessor GEM is a self-contained code that the user of FETCH interacts with directly. GEM will process an input file generated by the user. GEM will then generate a mesh then process the materials and the options. GEM can generate structured and unstructured mixed meshes using established algorithms such as Advancing Front and Delauney triangulation. The geometry capabilities are very general being formed from points, straight lines and region definitions within the input file by the user. The general basic geometry input entered in text files however can lead to input files that are excessively large (of the order of 10,000 or 100,000 lines of input). As with the output analysis component only verification need be considered for GEM. Solution and code algorithm verification is necessary with regard to algorithms associated with mesh generation. This is achieved
by expert users visualising the mesh generated before being used within the EVENT and/or FLUIDITY components. Verification has also involved comparison of the mesh data with other codes in the past. A range of error checkers exist within GEM such as detecting negative volumes or incorrectly defined regions. SQE practices have involved the use of debugging tools such as GDB and Valgrind. GEM is effectively a frozen code in that no future development is envisioned. Any V&V test case that runs the FETCH code implicitly includes an inferred verification test of GEM. In general no V&V documentation of GEM exists and it is regarded the users responsibility to deduce reliability. This is clearly not rigorous V&V and is an issue being solved through the development of a new user interface within the AMCG in an open source community. This new interface is however not linked with the current FETCH.

EVENT functions as an independent code but is heavily reliant on the preprocessor GEM for general usability. Ideally verification of GEM, already discussed, is therefore a prerequisite to EVENT V&V, however it is often inseparable. In the past basic unit tests were performed on key individual parts of the EVENT code however no documentation of this exists. In general no V&V documentation exists for EVENT. EVENT verification has relied heavily on literature benchmark problems. These have focused on criticality and shielding (fixed source) benchmark types where the reference solution is usually taken to be a Monte Carlo solution. These have been peer reviewed in the literature de Oliveira (1986), Ziver et al. (2005), de Oliveira et al. (2001) and Keller and de Oliveira (2004). These benchmark cases provide inseparable evidence of solution and code verification of both EVENT and GEM. SQE practices have been routinely employed in the development of EVENT to maintain code verification. Further solution verification can be inferred from the argument that the underlying mathematics embodied within EVENT is based on established numerical techniques (such as FEM, spherical harmonics and Conjugate Gradient Solvers). With regard to the time dependent discretisation within EVENT a widely established method is used and therefore solution verification is inferred from this. Code verification for time dependent simulations was only weakly justified through application to complex FETCH validation cases for fissile solutions. This is clearly not rigorous V&V for time dependent problems and is an issue that is investigated in later sections of this chapter. Of particular concern with
regard to the suitability of peer reviewed EVENT V&V papers to provide evidence is that before the process in the following section (automated V&V) started there were effectively three EVENT codes in existence. These are named EVENT-2 EVENT-3 and EVENT-4. It is not immediately obvious which version of EVENT was used for the benchmarks published in the literature. EVENT-2 was the version within FETCH, EVENT-3 was the last version from the main developer while at Imperial College and EVENT-4 is the latest version from the main developer after leaving Imperial College. EVENT-4 is not relevant to this research and any V&V associated with this version is not applicable. The issue associated with the existence of EVENT-2 and EVENT-3 was resolved through the automated V&V process described in the following sections to leave one EVENT associated with FETCH. As a part of this process new time dependent benchmarks were analysed to provide evidence of verification. Also as a part of this recent V&V process a substantial amount of the EVENT code was reviewed by experts for correctness of implementation.

FLUIDITY also functions as an independent code but is also (for use within FETCH and multiphase flow) heavily reliant on the preprocessor GEM for general usability. Therefore, as for EVENT, verification of GEM would be the ideal prerequisite but is often an inseparable process. FLUIDITY is a substantially larger code than EVENT and in the past decade has had a rapid increase in developers and users. Verification has included in the past general good SQE practices such as the use of debugger tools like Valgrind and numerical algorithm inspection by several experts. Solution verification has also been applied through application to standard CFD test cases such as flow past a cylinder. In the past five years due to an increase in research funding associated primarily with ocean modelling, FLUIDITY has undergone major software re-engineering. The purpose of this included:

1. Best programming practices such as modularity, standardisation, portability and documentation.
2. Dynamically allocatable memory.
3. Alternative model input (not GEM) for easier and more rigorous usability.
4. Linking with new efficient solver libraries such as PETSc.
5. Improved documentation for developers and users.

6. Inclusion of automated V&V test cases that include proper unit tests.

The latter point included the development of a framework Farrel et al. (2009) to perform the automated V&V which is described in the next section. A large number of test cases were produced which included substantial unit tests, solution verification tests and numerical algorithm test cases. Due to the focus of the researchers all these test cases were directed at either single phase or multimaterial problems. None were explicitly formed for Computational Multiphase Fluid Dynamic (CMFD) or coupled FETCH problems. However, many of the input, assembly, solvers and output routines within FLUIDITY are generic such that this verification process also provides evidence for multiphase and FETCH applications also. This process continued until the start of 2009 when due to time constraints project management decisions resulted in the FLUIDITY code associated with FETCH being branched. This resulted in two FLUIDITY codes, one associated with FETCH and one not. The automated V&V process continued on the main ocean FLUIDITY but ceased on the FLUIDITY branch associated with FETCH. Verification of the FLUIDITY branch associated with FETCH is therefore still strongly dependent on the user having the expertise to deduce correctness for FETCH specific cases.

Verification of the FETCH code is generally inferred through verification of the components separately and is considered adequate. Code that is specific to the FETCH interface has had the same SQE practices applied as to EVENT and FLUIDITY. Solution verification of FETCH has not been performed primarily due to the complexity of the multiphysics model. Analytic solutions and MMS are not known for coupled RT-CMFD problems (apart from perhaps point kinetic model solutions) and thus solution verification relies on code to code comparison. FETCH is however unique in its capabilities to model complex RT-CMFD problems such as fissile solutions implying that code to code comparison is extremely difficult to achieve. It is however possible to compare a subset of the FETCH capabilities with other coupled codes for solution verification. For example industrial established reactor kinetics codes such as PANTHER can provide a comparison for problem types using diffusion theory in EVENT and extremely simplified thermal models within FLUIDITY. This proposition is exploited in the proceeding sections.
to produce simplified verification test cases.

As stated in the previous section rigorous validation of a large multipurpose multiphysics model such as FETCH is extremely difficult. A couple of cases of validation of EVENT are known for shielding applications of the ASPIS experiment WARNER and DE OLIVEIRA (2000) and Dounreay reactor ZIVER et al. (2004). Here agreement of fluxes was within 20%. These were not only a validation of the EVENT code but also the nuclear data libraries used for the materials. It is therefore difficult to deduce the cause of the 20% error. EVENT was applied to the critical experiments GODIVA, JEZEBEL and OY-C with the results presented in the original thesis de Oliveira (1986). This involved a comparison with highly accurate reference solutions produced using 6 group Hansen Roach cross sections and an Integral Transport Code FLUBAG. This was a verification test of EVENT in spherical, RZ and XYZ geometry. A validation test was then presented using the same geometries but with improved cross sections (that included a P3 scattering kernel) that were collapsed from 100 group libraries to 6, 12 and 24 groups. The validation test compared the EVENT Keff to the inferred experimental value of 1.0 (being critical experiments). For GODIVA with EVENT P3 scatter kernel using 24 energy groups a Keff of 1.000134 was calculated. EVENT has also had validation in the prediction of critical heights of fissile solutions such as SILENE Pain et al. (2001a). Certain automated test cases discussed previously that were applied to the FLUIDITY within FETCH for single phase flow were considered validation cases but no documentation of them exists. FETCH as a whole has been compared to certain fissile solution criticality accidents and controlled experiments of transients Pain et al. (2001a) and Pain et al. (2001b). Comparisons were made to globally integrated system responses such as power and over pressure, as well as local system responses such as temperatures at detector locations. Agreement was presented to be within 30%. These validation comparisons implicitly involved a validation of the cross section generation by the WIMS code also. FETCH in these applications has provided a theoretical explanation of the dynamics detected in the experiments, such as power oscillations induced from free surface sloshing.
3.4. AMCG Continuous Quality Assurance Set Up

This section describes the framework used to assert continuous V&V evidence in a computationally practical manner. This framework is a recent innovation within the AMCG and this section draws largely from the internal reports Farrel et al. (2009) and Pain et al. (2008a).

A computational code representing the implementation of a mathematical model can be in a continuous state of simultaneous development and usage for a significant period of time (perhaps decades). Also the hardware and other auxiliary software (such as compilers) on which the code is dependent is also continuously evolving. This implies that the Quality Assurance process (which includes V&V) should adapt to the changing code, developers and user base. The ability to reproduce credible evidence to support V&V is a necessity, especially if high consequence decisions are expected to be made from model solutions and predictions. The strongest statement in this respect is to assert that any change of state associated with the code negates any previous V&V evidence. This argument then implies that all V&V evidence gathering would need repeating. The amount of work (computationally and human) associated with the V&V process is demanding. The computational work needed for repetition can be justified as a necessity. The human work needed for repetition of V&V should be minimised to reduce human error and be economically competitive. The human work involved (being the deducement of correctness, error and accuracy to within a subjective tolerance) in the initial V&V process can be computationally automated to produce a report of the state of V&V evidence. This repetition of V&V evidence gathering would be triggered into action from each occurrence of code change. If no code change is actually occurring but the code is still heavily used then it is still beneficial to have the V&V evidence gathering repeated at periodic intervals (such as daily or weekly) as the hardware and auxiliary software may well be changing. Figure 3.2 illustrates the automated V&V process in the context as to being applied to FLUIDITY alone.

The source code is managed by a Source Code Control System (SCCS) such as the open source Subversion (SVN) Subversion. The SCCS maintains all the revisions resulting from changes made to the code. Log files written by developers about changes to the code provide human readable summaries to
Figure 3.2.: Simple schematic of the automated V&V process Farrel et al. (2009) applied to FLUIDITY.
inform all the developing team. Developers check out a copy of a particular revision of the code, make changes as needed locally to their own copy then commit these back to the main repository controlled by the SCCS. The SCCS is flexible in that the code can be branched and merged as needed, simultaneous changes can be made by multiple developers and changes can be reverted if desired. The SCCS can be linked to an email group and website such that log files associated with repository commits can be shared instantly and effectively with the developing team. This provides immediate traceability and accountability to code repository changes. The SCCS is also importantly very simple to learn to use through a few commands.

The SCCS notifies the Software Development Continuous Integration Tool (SDCIT) when code repository changes occur. The SDCIT used for automated FETCH V&V is the open source program Buildbot Buildbot. The SDCIT contains a configuration script with a set of instructions (the buildmaster). This configuration script can initiate similar scripts on a range of chosen machines (buildslaves). The buildslaves will initially compile the code on the range or platforms on which they are installed. If unsuccessful the process stops for the particular buildslave and an email notification is sent as well as the website updated. Typically buildslaves will cover a range of machine architectures and compiler flag options.

If the code compile is successful the buildslave then initiates the unit tests. Unit tests check individual components of the code and are associated with verification. They perform automatically what is usually performed by a developer in checking the correctness of each code block by eye balling printed output. Unit tests were incorporated into FLUIDITY but not into GEM or EVENT. Unit tests can be applied to every individual function or subroutine associated with FORTRAN programming. They are typically very fast tests to perform. If the Unit tests fail then the automated process stops and developers notified. If successful the test cases associated with the buildslave are initiated.

Test cases involve running the entire compiled code on a predefined problem. Typically test cases are grouped together on the time taken to perform them (such as short tests, medium tests and long tests). Other test case classification can be useful such as to distinguish the problem types. For example the test cases developed for EVENT were grouped also into eigenvalue, fixed source and time dependent. Each buildslave after the unit test
phase runs a predetermined order of groups of tests. This allows simultaneous testing of different problem types or a sensible chosen order. For example one buildslave associated with FETCH would run EVENT short tests, another would run EVENT medium tests, another FETCH short tests and yet another FETCH medium tests. The test groups were each run in the order of fixed source, eigenvalue then time cases. Emphasis is determining code change errors as rapidly as possible. Test cases involve input files, reference solutions (which could be tabulated or a function within a script) and then scripts to extract the output solution, compare to the reference and then to assert a pass, warning or failure. The framework developed within the AMCG used XML and Python scripts for the latter point. Passes, warnings and failures are reported as needed to developers. Grouping the tests allows the process to be terminated if a failure is detected within a group such that developers do not have to wait for all tests to run.

This automated V&V process has the benefit that immediate feedback to changes in correctness, error and accuracy (which could be positive or negative) is provided. If failures are detected they can be managed effectively as the intention of changes are fresh in the mind of developers. The process also provides direct traceability and accountability as to which developers have caused unintended issues. This aids in avoiding the situation where developer A introduces code changes that have unintended effects to developer (or user) B’s research. If code errors are introduced and are unable to be corrected then the SCCS can be used to revert the changes by any developer. Also if a test case is introduced that relies on code that has been within the repository for substantial revisions and initially does not pass but is considered to have been possible in previous revisions, automated scripts can be used to run the test case through each past revision until a pass is obtained. The SCCS can then be used to determine the changes between the pass and fail revisions. As with any V&V process the greater the number of tests the greater the amount of evidence supporting credibility and reliability conclusions.
3.5. FETCH Automated Verification and Validation Test Case Suite

This section describes the automated FETCH V&V test case suite that was developed as part of this research. Other research projects within the AMCG initiated a similar process solely for FLUIDITY which was discussed in the previous sections. The framework developed from this was then applied to EVENT and FETCH. The purpose was to produce one EVENT associated with FETCH with the ability to provide up to date V&V evidence that is credible and reliable. Emphasis focused on verification as this should always be performed first. As the code was being tested primarily by the author who had little experience with the actual coding structure and style unit tests were simple impractical. Testing could only be achieved through actually running the combined GEM-EVENT codes on problem cases. This therefore encompassed software quality engineering, algorithm and solution verification in each test.

Test cases were constructed and applied to both EVENT-2 and EVENT-3 at first. The two versions of EVENT generally agreed for eigenvalue and fixed source problems. However for time dependent problems differences arose. Changes that were made to EVENT-2 to incorporate it into FETCH were introduced into EVENT-3 and this was used as a base for development. Previous applications of EVENT codes published within the literature were considered as well a range of other cases that were obtained from the literature with an emphasis for analytic solutions. For time dependent problems with delayed neutrons and some sort of thermal feedback, simple test cases were not found within the published literature. Therefore comparisons were made as best as possible with the industrial certified nodal kinetics code PANTHER. Comparison were made for simple test cases defined by the author. Comparisons for time-delayed-thermal feedback problems were also made between EVENT and a point kinetics code (PK) constructed by the author. During the assessment of the EVENT spatial FEM solver it was found necessary to compare to an independent 1D FEM diffusion code made by the author (developed originally for the thermal submodels for modelling the heterogeneity of a VHTR). This 1D FEM code evolved eventually into a 1D, 2D or 3D multigroup FEM neutron diffusion code combined with the point kinetics code such as to be able to solve eigenvalue and time dependent
problems.

This code was called BEANS and formed the basis for the Sub Grid Scale methodology developed in the proceeding chapter. BEANS was produced primarily by the author with the support from AMCG researchers. Most of the code was written fresh with a handful of subroutines taken from FLUIDITY. BEANS was linked with the solver library PETSc for increased performance and was developed within the automated test framework. BEANS uses standard Lagrange linear or quadratic finite elements, power iterations, outer iterations, multigroup sweeps, theta time stepping with rebalance acceleration and established Conjugate Gradient algorithms for the inner energy group solve. The methodology is therefore standard and the code is suitable for inter comparison with EVENT, with EVENT using its lowest angle approximation for the solution and scatter kernel. BEANS is capable of using a mesh generated by GEM or GMSH with each providing region (volume and surface) identification numbers which are then associated with material and boundary condition (being reflect, vacuum and zero) mappings. The options and material properties input is read separately and has nothing to do with GEM. Output from BEANS includes region averages, time series data and spatial flux distributions that can then be visualised within PLOTTER, PARAVIEW or GMSH.

Developments to the BEANS code that occurred during this research included:

1. Inclusion of anisotropic diffusion coefficients in the coordinate axis directions.

2. Inclusion of a range of Flux Limited Diffusion (FLD) coefficients.

3. Link with the optimised PETSc solver library allowing the use of a range of reliable solvers and preconditioners.

4. Spatial distribution output at specified time intervals, similar to FLUIDITY.

5. Time series output, similar to FLUIDITY.

6. Whole domain within group (as opposed to all group) rebalance acceleration (later included into EVENT).
7. Development of a Control Rod movement algorithm for structured meshes in the z axis for eigenvalue and time dependent problems (later partially included into FLUIDITY).

8. The ability to initialise a time dependent problem with a previous eigenvector solution, normalised as necessary (later included into EVENT for strictly diffusion angle approximation).

9. The ability to normalise the eigenvector solution to arbitrary total fission, power or flux with or without the Keff as a factor (later power normalisation included into EVENT).

10. Homogenisation (spatial and energy) routines that included a Super Homogenisation method (SPH).

11. A Sub Grid Scale (SGS) diffusion methodology.

12. The option to use element wise or discontinuous basis functions of the same order as the flux solution to resolve the spatial distribution of the delayed neutron precursors.

13. Inclusion of the delayed neutron precursor spectrum term in the eigenvalue calculations as necessary (later included into EVENT).

14. Dynamic memory allocation as well as other modern FORTRAN features such as fully modular and data types.

15. The option to store the block matrix associated with each energy group involved in the solver sweeps. Matrix assemble thus need only occur once for an eigenvalue calculation or per time step.

16. The option to store the integrated spatial tables or calculate one element at a time as needed.

17. The option to store the element wise interpolated material data set or calculate one element at a time as needed.

18. The option to exit the power iteration loop checking the Keff convergence only or to persist until the eigenvector has also converged to a prescribed tolerance. The former was the EVENT default until the latter was included as an option also.
19. The ability to have ramp changing absorption cross sections associated with certain materials for time dependent problems.

20. The ability to have energy group dependent flux extrapolation as the initial guess for each time step.

21. The inclusion of a simplified thermal equation (called miniFLUIDS) for simple feedback (also included into EVENT).

22. Generic coding such as to allow linking with alternative mesh generators to GEM such as GMSH.

23. The ability to perform coupled eigenvalue, FLUIDITY (or miniFLUIDS) and control rod movement simulations.

24. The ability to initialise an eigenvalue problem using a FLUIDITY (or miniFLUIDS) input state (also included into EVENT).

25. The ability to perform forward then adjoint mode calculations and to use these solutions to determine model parameters associated with the point kinetic equations.

26. The ability to perform radiation-fluids or fluids-radiation calculations within a time step (also included into EVENT).

BEANS was further linked with the FLUIDITY version that EVENT is linked with. For the sake of distinguishing them FETCH-E refers to the coupled codes EVENT-FLUIDITY and FETCH-B refers to the coupled codes BEANS-FLUIDITY. In the proceeding chapters both FETCH-E and FETCH-B are used. Both BEANS and EVENT therefore require verification evidence. During the process of performing this automated V&V on the EVENT code errors associated with software engineering or algorithm implementation were discovered. Mostly these were found to have minor (if any) noticeable consequences for test cases similar that which FETCH-E has been applied to in the past. For example with certain input combinations the fixed source in time dependent problems was found to be included twice. A trivial error for FETCH-E applications where a very small source is solely used to initiate the transient but a detrimental error for simplified problems desired for automated test cases. A non trivial error was discovered associated with the explicitly delayed neutron precursors calculated in
FLUIDITY being added into the EVENT source. This was subsequently rectified and maintained through a simple test case. This is highlighted to emphasise the benefit of automated V&V as this error had appeared after being used correctly and published within the literature.

Just over one hundred test cases were created for FETCH-E with around 80% having been produced by the author. Most were simple enough such as to run to completion in seconds. Also, tessellation of test cases such as to be represented in different geometries or meshes was exploited. Just under 10% of the FETCH-E test cases were fixed source problems with the rest split evenly between eigenvalue and time dependent problems. Most of the test cases are classified as verification. The few validation test cases included within the V&V framework were either SILENE or TRACY fissile solution criticality problems similar to that analysed in the FETCH literature. Verification GODIVA test cases were also included but not analysed as validation. It was found that for test cases that had previously been published in the literature the current FETCH-E was capable of reproducing practically the same results. These test cases included GODIVA, TAKEDA 1B Case 2, SILENE, TRACY, three cases (two fixed source and one eigenvalue) compared to the analytic solutions in Williams (2005) and a RZ time dependent case compared to TWODANT de Oliveira (1990). Over 20 test cases from the analytic benchmark set Sood et al. (2003) were included. The analytic diffusion solution for a surface source on a non multiplying slab from Stacey (2007) was included in 1D, 2D and 3D geometry models. Four analytic solutions test cases from Olson and Henderson (2004) for time dependent problems were produced. These included infinite, slab and spherical problems in non multiplying media that required a transport solution. For multiplying media test case comparisons were made for simple infinite (all reflect) problems of the time constant with the analytic solution. This included with and without delayed neutrons. A build up of complexity of time-delayed-thermal feedback test cases were then defined and produced. This included infinite (all reflect) cases compared to PANTHER and a simple point kinetics code for implicitly and explicitly (either miniFLUIDS or FLUIDITY) coupled delayed neutrons. Two group cross sections and delayed data were used characteristic of a LWR fuel assembly taken from a literature benchmark. A 1D slab test case with the same material properties for time-delayed-thermal feedback was then compared to a separate
small 1D code. Similarly a simple 2D square and 3D cube test cases were included and compared to PANTHER and BEANS. For each of these cases the power and maximum temperature with time were compared. Generally agreement was with 1%. Two time-delayed whole core test cases in 2D geometry from the benchmark book ANL-7416 (1977) were also included. These two cases were part of the V&V tests supplied with the PANTHER code and PANTHER was thus used as the reference as well as literature values. Differences of the total power with time were less than 0.1%. Slight variations of these last test cases were produced via changing the zero boundary condition to vacuum and increasing the number of delayed groups from one to six. PANTHER again was taken as the reference with agreement within 0.1%. Note that all the verification time-delayed-thermal feedback test cases had a neutron diffusion reference. None requiring actual neutron transport solutions were implemented as all encountered within the literature were diffusion based.

The FETCH-E test cases covered the following:

1. Slab, cylindrical, spherical, XY, RZ and XYZ geometries.
3. One group and multigroup problems.
4. Structured and unstructured meshes, including mixed mesh domains.
5. Reflect, vacuum, zero and prescribed isotropic source boundary conditions.
6. One material and multimaterial problems, including almost void conditions.
7. Strict diffusion, P1 and Pn angular expansions.
8. Isotropic and anisotropic scatter kernels.
9. Use of the two functioning within group solvers.
10. Implicitly and explicitly coupled delayed neutron precursor equations.
11. Different shape functions (line, triangle, quadrilateral, wedge, tetrahedral and hexahedral).
12. Linear and quadratic order shape functions where functioning correctly.

13. Fully implicit (theta 1.0), Galerkin (theta 0.666) and Crank Nicholson (theta = 0.5) time stepping for the flux and delayed equations.

14. Fixed time stepping and adaptive time stepping that can change through time zones.


17. Eigenvalue runs initialised by FLUIDITY or miniFLUIDS state.

18. Normalisation of the eigenvector to a designated total power.

19. Initialisation of a time dependent run with a normalised eigenvector solution.

20. Use of the control rod algorithm in eigenvalue (as initialisation) and time dependent runs (inducing a ramp material change).

21. Use of rebalance acceleration or not.

The FETCH-E test cases compared the following output to the various references:

1. Eigenvalue.

2. Volume region average fluxes.

3. Point fluxes.

4. Total power.

5. Surface region leakage.

6. Maximum temperatures.

The FETCH-E tests cases were compared to the following types of reference solutions:

1. Analytic.
2. Monte Carlo.

3. Point kinetic code.

4. 1D FEM diffusion code.

5. 3D FEM diffusion code BEANS.

6. Sn transport code TWODANT.

7. Nodal diffusion code PANTHER.

8. Experimental measurements of SILENE and TRACY critical fissile solutions.

Around 30 test cases were produced for BEANS. Most of these were also within the EVENT tests. This included eigenvalue and time dependent problems such as the point kinetic, slab, square, cube and the whole core benchmark ANL-7416 (1977) cases that were compared to PANTHER. Generally numerically identical agreement was observed between EVENT and BEANS for these cases. This is expected as they are theoretically identical in certain circumstances. A simple square domain RZ diffusion test case was used to verify BEANS via comparison with EVENT, which had RZ transport test cases such as GODIVA for verification. A simple cube problem with anisotropic diffusion coefficients was used to verify BEANS via comparison with PANTHER. In each of these two cases numerically identical agreement was found for converged mesh solutions. Simple cube problems were also used as regression tests for maintaining what was considered sensible results for the coupled eigenvalue, control rod and miniFLUIDS algorithm. The TAKEDA1B case 2 benchmark was used as a 3D test compared to EVENT (which had been verified for transport solutions) for hexahedral, tetrahedral and prism shape functions. This last test also included the use of the control rod algorithm to place the rod but not move it. An eigenvalue test case from the benchmark book ANL-7416 (1977) of a whole core BWR in 2D was included and compared to PANTHER and EVENT for the power densities and fluxes respectively. This test case was also used to investigate the Sub Grid Scale diffusion methodology developed that is presented in a proceeding chapter. Finally one validation test case was included for the HTR-10 pebble bed reactor to find the initial critical height and is presented...
in a proceeding chapter. On top of the 30 test cases outlined over an extra 50 were produced associated with the whole core VHTR modelling of proceeding chapters. Many were set up to capture the various stages of the VHTR specific model development as regression tests. Some also included inter comparisons such as RZ to XYZ as well as comparisons to EVENT and the Monte Carlo code MONK9. Some of these test cases included coupled FLUIDITY or miniFLUIDs simulations for eigenvalue or time dependent problems. In summary the FETCH-B test cases covered the following:

1. Slab, XY, RZ and XYZ geometries.
2. Fixed source (via one large implicit time step), eigenvalue, time, time-delayed, time-delayed-thermal, time-delayed-CMFD feedback problems.
3. One group and multigroup problems.
5. Reflect, vacuum and zero boundary conditions.
6. One material and multimaterial problems.
7. Use of the Gauss Seidel, Conjugate Gradient and PETSc solvers.
8. Implicitly and explicitly coupled delayed neutron precursor equations.
9. Different shape functions (line, triangle, quadrilateral, wedge, tetrahedral and hexahedral).
10. Linear and quadratic order shape functions where functioning correctly.
11. Fully implicit (theta 1.0), Galerkin (theta 0.666) and Crank Nicholson (theta = 0.5) time stepping for the flux and delayed equations.
12. Fixed time stepping and adaptive time stepping that can change through time zones.
14. Coupled FLUIDITY and miniFLUIDS for eigenvalue and time dependent problems.
15. Eigenvalue runs initialised by FLUIDITY or miniFLUIDS state.

16. Normalisation of the eigenvector to a designated total power, total fission or total flux.

17. Initialisation of a time dependent run with a normalised eigenvector solution.

18. Use of the control rod algorithm in eigenvalue and time dependent runs.

19. Use of ramp materials.

20. Use of rebalance acceleration or not.

21. Forward and adjoint problems followed by calculating point kinetic parameters.

22. Adjoint verification via comparison with appropriately modified forward solution input.

23. Spatial and energy homogenisation via SPH method.

A selection of test cases are next presented in more detail with an emphasis for time dependent verification problems. All macroscopic cross sections are given in units of cm$^{-1}$, spatial dimensions units in cm and time dimension units in seconds. Unless stated it should be assumed that the isotropic transport cross section is given by

$$\Sigma_{trg} = \Sigma_{tg}$$

(3.1)

and that the isotropic diffusion coefficient used is given by

$$D_g = \frac{1}{3\Sigma_{trg}}.$$  

(3.2)

Errors are compared for order of convergence where the order is deduced via comparison of gradients with functions given by

$$f(x) = kx^{-N},$$

(3.3)
where $k$ is an arbitrary constant taken as 1.0 and $N$ is the integer being the order of convergence. Unless stated it should be assumed that solver (inner and outer) tolerances were set to $1.0E-08$.

### 3.5.1. Infinite Non Multiplying Media Time Dependent

This test case consists of a infinite (all reflective) non multiplying media with a fixed source. This is a time dependent problem with an initial one group flux of zero. The reference solution is given by the analytic solution Olson and Henderson (2004)

$$
\phi(t) = \frac{S_0}{\Sigma_a} \left( 1 - e^{-\Sigma_a v t} \right),
$$

(3.4)

where $\phi$ is the flux solution, $S_0$ is the prescribed constant source, $\Sigma_a$ the absorption cross section, $v$ the one group neutron speed and $t$ the time.

The values used for this test case are given in table 3.1. This test case was modelled in 2D (XY and RZ) and 3D geometry using all reflective boundary conditions in both EVENT and BEANS. Cases were modelled using adaptive and fixed time stepping. The fixed time step size was varied through different time zones. The time discretisation (theta value) was also varied within the same simulation through time zones to cover fully implicit, Galerkin and Crank Nicholson schemes. The flux was compared at 0.1sec, 1.1sec, 11.1sec, 111.1sec and 1111.1sec. Agreement between EVENT and BEANS to the analytic solution was within a relative tolerance of $1.0E-06$. The temporal convergence of the different theta schemes was analysed via comparing the relative error at 0.1sec using a range of number of fixed time steps taken. These results are illustrated in figure 3.3 where the expected convergence of theta equal to 1.0 and 0.5 are observed.

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<th>$\Sigma_t$</th>
<th>$\nu \Sigma_f$</th>
<th>$\Sigma_s$</th>
<th>$\Sigma_a$</th>
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Table 3.1.: Material properties and source strength of the test case Infinite Non Multiplying Media Time Dependent.
Figure 3.3.: Temporal convergence for different theta value methods for the test case *Infinite Non Multiplying Media Time Dependent.*
3.5.2. Infinite Multiplying Media Time Dependent

This test case consists of an infinite (all reflective) multiplying media in 2 energy groups with 1 delayed precursor group. This is a time dependent problem that is initialised by a normalised to one unit power eigenvector solution. Simple thermal feedback through linear interpolation between the material at two temperatures is used. The difference between the material properties for the two temperatures is an increase in fast group absorption at the higher temperature. Material properties are characteristic of a BWR fuel assembly taken from the LRA benchmark ANL-7416 (1977). As the geometry is infinite the $\nu\Sigma_f$ material numbers presented have been pre-divided by the Keff to avoid excessive reactivity. A step reactivity of $1.9743$ is induced at the start of the transient via a step change in the group 2 absorption cross section by $0.0010773$. The initial temperature is taken to be $500K$ and the duration of the transient is $1.0sec$. Results are initially compared to PANTHER for a fixed time step size of $1.0E−04$. PANTHER has what is considered a superior time discretisation that is analytic for the delayed (assuming a linear fission source in time) and exponentially transformed for the neutron flux. Time step size convergence for difference theta schemes is then analysed, where the reference solution is the solution for theta being $0.5$ with a time step size of $5.0E−06$. The material properties used are given in table 3.2. This test case was solved with both EVENT and BEANS which produced practically identical solutions.

The power and temperature maximum relative errors for a fixed time step size of $1.0E−04$ for different time schemes are shown in table 3.3. Here the same time scheme is used for the neutron flux and delayed precursor equations. For a fixed theta associated with the neutron flux discretisation the results were found to be insensitive to the theta associated with the delayed precursor discretisation. The 0.5 theta value has a solution error an order of magnitude lower than the 1.0 theta value discretisation for this temporal resolution. The 0.666 theta value reduces the solution error by about a half compared to the 1.0 theta value solution. Figure 3.4 shows the power evolution for the different theta methods on logarithmic axis scales. From this resolution of graph to graph analysis it is not obvious that a 5% difference exists which highlights the necessity to directly process each time step result rigorously.
Figure 3.4: Power evolution for different theta value methods for the test case *Infinite Multiplying Media Time Dependent*. Note that the three graphs are practically indistinguishable.
To analyse the temporal convergence in more detail the relative error of the maximum power achieved for the different theta methods is compared. Again the same theta value is used for both the neutron flux and delayed precursor equations. The results are presented in figure 3.5. The theta 0.5 solution has a second order convergence as expected. The theta 1.0 and 0.666 solutions have a first order convergence as expected with the theta 0.666 giving the more resolved solution of the two. Finally it was observed that for larger time steps, or values of theta, the neutron population increased more rapidly and obtained a larger power.

3.5.3. TWIGL 2D Time Dependent

The TWIGL Song and Kim (1992) benchmark problems are a simplified 2D time dependent code to code comparison verification tests for diffusion kinetic models. This test case is used to provide verification evidence of spatial and temporal convergence of EVENT and BEANS for a multimaterial finite
problem. Results from EVENT and BEANS for this test case were found to be practically numerically identical for identical model set up as expected. The geometry consists of seed and blanket regions characteristic of a PWR core of 20 by 20 fuel assemblies of size 8cm by 8cm. The geometry has a octant symmetry and is modelled as a quarter core. Two neutron energy groups and 1 delayed precursor group are used. The time dependent simulation is initialised by the normalised eigenvector solution and the $\nu\Sigma_f$ cross sections divided by the $K_e$ such as to be critical. A delayed super critical transient is then initiated via a change in the group two absorption cross section of material 1 (that forms part of the seed region) by $0.0035 \text{ cm}^{-1}$ either as a step or a linear ramp over 0.2sec. The transient is simulated for 0.5sec and power compared at 0.1sec intervals. Reflective boundary conditions are used to capture the symmetry and zero flux boundary conditions are used on the outside of the model domain. No thermal feedback is included with in the benchmark description. The reference solution is taken as that given by the finest spatial and temporal discretised results given by the code SPANDEX in Sutton and Aviles (1996). SPANDEX is a Nodal Expansion Method (NEM) code and was shown in Sutton and Aviles (1996) to be within $1.0E^{-3}$ relative error accuracy to four other nodal codes (being CONQUEST, QUANDRY, PANTHER and CUBBOX) with regard to the power for this test case. SPANDEX is thus deduced to have reliable and credible evidence such as to be suitable to provide the reference solution for this comparison.

The material properties for this test case are shown in table 3.4. The initial time dependent flux is normalised to unit power and the heat released per fission $w$ used is 1.0 (which is arbitrary for this test case). The geometry and material mapping are shown in figure 3.6. Spatial and temporal convergence of the global $K_e$ and transient power are analysed.

The spatial convergence of the $K_e$ for linear and quadratic basis functions is shown in figure 3.7 using a logarithmic axis plot and is also shown in table 3.5. The linear basis function solution is observed to have a second order convergence and the quadratic a corresponding third order as expected. Ten element divisions in the each axis direction corresponds to one element per fuel assembly of size 8cm by 8cm. With 80 elements in each axis direction the mesh is of size 1cm by 1cm giving 64 elements per fuel assembly. To converge the $K_e$ relative error to about 1pcm table 3.5 shows that linear
Figure 3.6.: Geometry, material mapping and boundary conditions for the test case TWIGL 2D Time Dependent.
Figure 3.7: Spatial convergence for the Keff for linear and quadratic for the test case *TWIGL 2D Time Dependent*.
basis functions required 80 divisions whereas quadratic required about 25 divisions (rough interpolation between 20 and 30). This corresponds to 6561 degrees of freedom (expansion coefficients) for linear and 2601 for quadratic (a 60% reduction).

To analyse the temporal convergence of different theta values a spatial resolution of 20 divisions in each axis direction with quadratic basis functions was used. The maximum relative error of the power to a reference solution at 0.1 sec (the transient turning point between the initial prompt jump and the expected exponential time constant rise) was then compared for different number of time steps up to 0.1 sec with theta being either 1.0, 0.666 and 0.5. The same theta value was used for both the neutron flux and delayed precursor equations. The reference solution was the power value from a FETCH run with theta being 0.5 and using 10000 time steps. This had a value of 2.06175 Watts which is comparable to the SPANDEX literature value of 2.062 Watts. Figure 3.8 shows the temporal convergence for different theta values. For the coarsest time step size shown the 0.5 and 0.666 theta solutions are less accurate than the 1.0 theta solution. This is because the 1.0 theta method is fully implicit whereas the other two are semi-implicit. The theta 1.0 and 0.666 solutions show first order convergence as expected while the theta 0.5 solution shows a mixture of second and third order convergence rates. A time step size of 1.0E-03 is asserted to be satisfactory with a relative error of about 1.0E-04 for each theta value. The power evolution for theta 0.5 is shown in figure 3.9 along with the reference SPANDEX point solutions. The FETCH and reference solution are indistinguishable from this perspective.

The TWIGL ramp results showed a similar behaviour with regard to convergence and error as the step results and need not be shown.

3.6. Conclusions

This chapter described the importance verification and validation is in determining the reliability and credibility of computationally implemented mathematical models. The definition of V&V considered the most useful from literature was stated and a review of processes involved in gathering evidence presented. The assertion was made that a continuously evolving computational model should have a continuously evolving quality assurance proce-
Figure 3.8.: Temporal convergence for the power at 0.1 seconds for different theta values for the test case TWIGL 2D Time Dependent.
Figure 3.9.: Power evolution for theta 0.5 for the test case \textit{TWIGL 2D Time Dependent} shown with the reference point solutions.
dure, which includes V&V. A framework for performing continuous V&V in an efficient manner was described that is flexible enough to be applied to any numerical model. An overview of previous V&V applied to the FETCH code was given. This included significant general verification test cases that were peer reviewed and published as well as the validation test cases in the area of criticality of fissile solutions.

Recognition was stated that verification was needed for all the components that form the FETCH model, including any preprocessing and post-processing tools. Test cases that run the GEM-EVENT-FLUIDITY codes were used to provide evidence of verification of GEM. Although not rigorous this was deemed acceptable and currently the only viable option. Verification of post processing tools is heavily reliant on user expertise and is achievable through the use of multiple tools to deduce correctness. Post processing tools used for FETCH output analysis include open source community developed projects providing a large effective peer review group.

The progress made on automatic V&V applied to the FLUIDITY version within FETCH was described. This predominantly focused in the areas of single phase or multicomponent flows but also included basic advection diffusion solver and unit tests. The evidence of FLUIDITY V&V in the context of multiphase flow and within FETCH thus must be extrapolated from test cases that are using some of the same subroutines and functions. Also this recent V&V applied to the FLUIDITY within FETCH ceased being automatic at the start of 2009 due to availability of resources to support it and should thus be considered historic V&V evidence rather than current.

Issues associated with the existence of multiple EVENT codes was resolved through automatic continuous V&V driven development with the outcome of one EVENT associated with FETCH. Over one hundred test cases were created to produce continuous automatic V&V evidence for EVENT covering a range of applications. More emphasis than previously was directed towards time dependent test cases with delayed neutrons as evidence here was lacking. A range of verification test cases of time dependent problems were analysed in more detail. This included comparisons to analytic solutions as well as what was considered highly reliable numerical solutions, such as that from the nodal kinetics code PANTHER. During the EVENT V&V process it was considered necessary to compare with a similar FEM based code. This led to the development of a 3D multigroup FEM based
neutron diffusion solver called BEANS which embodied standard theory and solvers. BEANS was developed within the automatic V&V framework with over thirty test cases and subsequently became a versatile tool for method development and was also linked to FLUIDITY to form a FETCH-B (with FETCH-E now referring to EVENT-FLUIDITY).

Future verification associated with FETCH should focus on incorporating unit tests into a neutronic solver, establishing more rigorous test cases and unit tests for a preprocessor code and developing more applicable test cases and unit tests for a version of FLUIDITY in the context of multiphase flow. These directions are currently a research goal within the AMCG and involve the development of new radiation transport solvers, preprocessors and a new multiphase FLUIDITY linked within FETCH. Future FETCH validation suggestions are more difficult to state as the process is more involved and dependent on observational and experimental data being available. Nevertheless, if the funding and expertise were available then specifically designed validation experiments for problems of direct interest are strongly encouraged for a model that is potentially used in high consequence decision making.
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<td>Beta</td>
</tr>
<tr>
<td>Lambda</td>
</tr>
<tr>
<td>$\chi_d$</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Thermal Data</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
</tr>
<tr>
<td>Heat Capacity</td>
</tr>
</tbody>
</table>

Table 3.2: Material properties at two temperatures of the test case *Infinite Multiplying Media Time Dependent*.

<table>
<thead>
<tr>
<th>Theta</th>
<th>Maximum Relative Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Power</td>
<td>Temperature</td>
</tr>
<tr>
<td>1.0</td>
<td>0.05533 0.00817</td>
</tr>
<tr>
<td>0.666</td>
<td>0.02228 0.00407</td>
</tr>
<tr>
<td>0.5</td>
<td>0.00586 0.00205</td>
</tr>
</tbody>
</table>

Table 3.3: Maximum relative error of the power and temperature for different theta values for the test case *Infinite Multiplying Media Time Dependent* compared to PANTHER.
<table>
<thead>
<tr>
<th>Material</th>
<th>1</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>$\Sigma_t$</td>
<td>2.3809524E-01</td>
<td>8.3333333E-01</td>
</tr>
<tr>
<td>$\nu \Sigma_f$</td>
<td>7.0000000E-03</td>
<td>2.0000000E-01</td>
</tr>
<tr>
<td>$\Sigma_{s\rightarrow 1}$</td>
<td>2.1809524E-01</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>$\Sigma_{s\rightarrow 2}$</td>
<td>1.0000000E-02</td>
<td>6.8333333E-01</td>
</tr>
<tr>
<td>$w \Sigma_f$</td>
<td>2.8806584E-03</td>
<td>8.2304527E-02</td>
</tr>
<tr>
<td>$\chi_p$</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Velocity</td>
<td>1.0E+07</td>
<td>2.0E+05</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Material</th>
<th>2</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>$\Sigma_t$</td>
<td>2.3809524E-01</td>
<td>8.3333333E-01</td>
</tr>
<tr>
<td>$\nu \Sigma_f$</td>
<td>7.0000000E-03</td>
<td>2.0000000E-01</td>
</tr>
<tr>
<td>$\Sigma_{s\rightarrow 1}$</td>
<td>2.1809524E-01</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>$\Sigma_{s\rightarrow 2}$</td>
<td>1.0000000E-02</td>
<td>6.8333333E-01</td>
</tr>
<tr>
<td>$w \Sigma_f$</td>
<td>2.8806584E-03</td>
<td>8.2304527E-02</td>
</tr>
<tr>
<td>$\chi_p$</td>
<td>1.0</td>
<td>0.0</td>
</tr>
<tr>
<td>Velocity</td>
<td>1.0E+07</td>
<td>2.0E+05</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Material</th>
<th>3</th>
<th>2</th>
</tr>
</thead>
<tbody>
<tr>
<td>Group</td>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>$\Sigma_t$</td>
<td>2.5641026E-01</td>
<td>6.6666666E-01</td>
</tr>
<tr>
<td>$\nu \Sigma_f$</td>
<td>3.0000000E-03</td>
<td>6.0000000E-02</td>
</tr>
<tr>
<td>$\Sigma_{s\rightarrow 1}$</td>
<td>2.3841026E-01</td>
<td>0.0000000E+00</td>
</tr>
<tr>
<td>$\Sigma_{s\rightarrow 2}$</td>
<td>1.0000000E-02</td>
<td>6.1666666E-01</td>
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<td>$w \Sigma_f$</td>
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<td>2.4691358E-02</td>
</tr>
<tr>
<td>$\chi_p$</td>
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<td>0.0</td>
</tr>
<tr>
<td>Velocity</td>
<td>1.0E+07</td>
<td>2.0E+05</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Delayed Data</th>
<th>Beta</th>
<th>0.0075</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lambda</td>
<td>0.08</td>
<td></td>
</tr>
<tr>
<td>$\chi_d$</td>
<td>1.0</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Table 3.4: Material properties of the test case TWIGL 2D Time Dependent.
<table>
<thead>
<tr>
<th>Number Elements in Axis</th>
<th>Maximum Relative Error Keff Linear</th>
<th>Quadratic</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>3.1622E-04</td>
<td>1.2588E-04</td>
</tr>
<tr>
<td>20</td>
<td>1.3563E-04</td>
<td>1.6916E-05</td>
</tr>
<tr>
<td>30</td>
<td>6.8785E-05</td>
<td>3.9773E-06</td>
</tr>
<tr>
<td>40</td>
<td>4.0639E-05</td>
<td>1.1716E-06</td>
</tr>
<tr>
<td>80</td>
<td>1.0481E-05</td>
<td>2.2611E-07</td>
</tr>
</tbody>
</table>

Table 3.5.: Relative error of the Keff for linear and quadratic basis functions for varying number of elements in each axis direction for the test case TWIGL 2D Time Dependent.
Chapter 4

NEUTRON DIFFUSION SUB GRID SCALE FINITE ELEMENT METHOD

Synopsis

A recently developed inner element sub grid scale finite element method is presented in the context of being applied to the multigroup neutron diffusion equation. The method aims to have the improved coarse mesh solution accuracy characteristic of Discontinuous Galerkin methods but with the computational effort more characteristic of Continuous Galerkin methods. The Galerkin Weighted Residual formulation is described as applied to a one group neutron diffusion, absorption and fixed source equation. The extension to multigroup neutron diffusion as well as criticality eigenvalue and time dependent problems is presented. Also, consideration to various methods of treating the inner element boundary integrals are explored with respect to stability and accuracy. A simplification of the outer domain boundary condition is described. The method is analysed for a range of test cases of increasing hierarchical complexity with the use of linear and quadratic Lagrange basis functions. Finally conclusions and future suggestions are given.
4.1. Introduction

The standard Continuous Galerkin (CG) is an established numerical method for the approximate solution of elliptic and parabolic equations Pepper and Heinrich (1992). The method does not suffer from numerical stability issues in this instance as occurs when applied to hyperbolic convection dominated problems. For steady state elliptic or parabolic problems the CG method will give an accurate and stable solution provided enough basis function resolution is used. This can be achieved by refining the mesh or increasing the
basis function polynomial order. However if the solution to be found contains strong gradients, which could for example occur at material interfaces, then the resolution required could become excessive. If one of the materials at the interface has a larger absorption coefficient relative to the other interface material and if insufficient resolution is used then the solution obtained could contain local oscillations that may be non-physical.

Alternatively the Discontinuous Galerkin (DG) method could be applied. The DG method by its nature permits the solution to be discontinuous at element element interfaces. This characteristic is considered to increase the solution accuracy in demanding regions of a problem for a more coarser mesh than is required for the CG convergence. However, the main drawback of the DG method is the increase in the number of unknowns. The DG method was originally developed for application to hyperbolic equations where the CG method is unable to provide a stable solution. The first occurrence of the method was in 1973 by Reed and Hill (1973) in the context of obtaining solutions to the first order Neutron Transport Equation. Since then the DG method has become widely developed and applied in many areas of numerical analysis for hyperbolic problems. The diversification of the DG method developed for hyperbolic problems to other areas of interest has led to the development of this type of DG method applied to equation sets that contain a diffusive term. The first occurrence of the evolution of the method in this direction is considered to be by Bassi and Rebay (1997) in 1997. Variations of the method soon followed with respect to the treatment of the element element interface integrals. One of the most researched methods to arise is the Local Discontinuous Galerkin (LDG) method Cockburn and Shu (1998) Cockburn et al. (2001) which is more stable than the original formulation by Bassi and Rebay (1997). Following the development of these various DG diffusion methods a unification of them was presented by Arnold et al. (2001). This not only introduced a unifying framework for the DG methods that stemmed from adaptations of hyperbolic DG schemes but also included within it Interior Penalty (IP) methods Arnold (1982). The IP methods were developed independently of hyperbolic DG methods and around the same time period. The IP method is a generalisation of earlier research that considered the application of Dirichlet boundary conditions through the use of penalty parameters. An analysis of the various DG methods for elliptic equations with regard to accuracy, consistency, conservation and stability is

As previously stated the main drawback of the DG method in comparison to CG is the increase in the number of unknowns. For example, for a finite element mesh consisting of linear hexahedral shape functions the increase in unknowns within the domain is around 8. Not only are the number of unknowns increased but the connectivity between them also increases. These would both imply a more demanding matrix system to solve for with respect to time take and computational memory. Therefore a method that aims to have the accuracy of the DG method combined with the computational effort of the CG method is desirable. Recently such a combined method was formulated and analysed by Candy (2008), called a Sub Grid Scale (SGS) method. Candy (2008) analysed the proposed SGS method in the context of a general advection diffusion equation and considered the case of no diffusion (pure advection). The case of no advection (pure diffusion) was not investigated. Candy (2008) and Buchan et al. (2010) then analysed the SGS method in the context of the solution of the Neutron Transport Equation and Navier Stokes Equations (including free surface flows).

The SGS method in general decomposes the solution into a global coarse scale and an inner element fine scale. The method was originally proposed by Hughes et al. (1998) as the Variational Multiscale (VMS) method. The VMS method uses bubble functions to enrich the solution. The bubble functions are defined as the solution to the homogeneous inner element problem and generally to vanish on element boundaries. The global coarse scale is represented in an identical manner to the CG method. As the bubble functions are defined element wise a static condensation procedure is performed to effectively eliminate the fine scales leaving a matrix system to be solved that resembles that of a CG system. Hughes (1995) showed that this SGS method provided a formal derivation of stabilisation techniques such as Petrov Galerkin formulations. The SGS method formulated by Candy (2008) is an extension of that of given by Hughes et al. (1998) in that the fine scale basis functions are not restricted to be defined as zero on element boundaries. To decouple fine scale solutions between elements a weak enforcement of a zero Dirichlet boundary condition is used. Therefore a static condensation procedure can be performed to effectively eliminate the fine scales. Thus the solution obtained from the SGS method of Candy (2008)
is naturally discontinuous and with the effective computational effort of the CG method.

Motivated by the performance and characteristics offered by the SGS method of Candy (2008) it was analysed in the context of the neutron diffusion equation. During this analysis it was found that alternative variations on the treatment of the diffusion term associated with the fine scales was needed. These variations share characteristics with those used within the DG schemes. The rest of this chapter is organised as follows: section 4.2 formulates the residual based SGS method to be analysed which closely resembles that given in Candy (2008), section 4.3 then analyses the method via numerical application to a range of test cases and finally section 4.4 states conclusions and future research suggestions.

4.2. Sub Grid Scale Formulation

In this section the sub grid scale formulation applied to a one group neutron diffusion, absorption and fixed source equation is derived. The formulation and notation follows closely that given by Candy (2008). A simplification with respect to the full problem domain outer surface boundary condition is then shown. Different methods of treating the inner element surface integrals that arise in the formulation with respect to a zero Dirichlet boundary condition then follows. The static condensation solution algorithm that solves for both scales is then described. Finally, the extension of the method to multigroup neutron diffusion as well as eigenvalue and time dependent problems is then presented.

4.2.1. Problem Definition

The initial equation to be considered is the one group fixed source isotropic neutron diffusion equation given by

\[- \nabla \cdot D(r) \nabla \phi(r) + \Sigma(r) \phi(r) = S(r) \quad \forall \ r \in \Omega, \quad (4.1)\]

where \( \nabla \) is the standard vector partial differential operator, \( D(r) \) is a spatially varying isotropic diffusion coefficient, \( \Sigma(r) \) is a spatially varying absorption coefficient, \( S(r) \) is a prescribed spatially varying fixed source, \( \phi(r) \) the spatially varying neutron flux solution and \( r \) represents a coordinate
point within the spatial domain given by $\Omega$. To form a well posed problem definition the following boundary conditions are considered

$$\phi(r) = 0 \quad \forall \ r \in \Gamma_Z,$$  \hspace{1cm} (4.2)

$$\mathbf{n} \cdot D(r)\nabla\phi(r) = 0 \quad \forall \ r \in \Gamma_R,$$  \hspace{1cm} (4.3)

$$\mathbf{n} \cdot D(r)\nabla\phi(r) + 0.5\phi(r) = 0 \quad \forall \ r \in \Gamma_V,$$  \hspace{1cm} (4.4)

where $\mathbf{n}$ is the unit outward normal of the boundary surface. The outer bounding surface $\Gamma$ of the spatial domain $\Omega$ is formed from the union of $\Gamma_Z$ representing the zero Dirichlet boundaries, $\Gamma_R$ representing the reflect Neumann boundaries and $\Gamma_V$ representing the vacuum Robin boundaries.

Equations (4.1), (4.2), (4.3) and (4.4) can be more compactly written as

$$\mathcal{R}(\phi) = \mathcal{L}(\phi) - S(r) = 0 \quad \forall \ r \in \Omega,$$  \hspace{1cm} (4.5)

$$\mathcal{K}(\phi) = \mathcal{M}(\phi) = 0 \quad \forall \ r \in \Gamma,$$  \hspace{1cm} (4.6)

where $\mathcal{R}(\phi)$ is the volume residual as a function of $\phi$, $\mathcal{L}(\phi)$ is the volume differential linear operator containing the diffusion and absorption terms as a function of $\phi$, $\mathcal{K}(\phi)$ is the surface boundary condition residual as a function of $\phi$ and $\mathcal{M}(\phi)$ is the surface boundary condition linear operator as a function of $\phi$. The operator $\mathcal{M}$ takes different forms for the different types of boundary conditions.

### 4.2.2. Spatial Discretisation

The problem spatial domain $\Omega$ is partitioned into a finite number $n_{ele}$ of non-overlapping sub domains (or elements) $\Omega_{ele}$ such that

$$\Omega = \bigcup_{ele=1}^{n_{ele}} \Omega_{ele}.$$  \hspace{1cm} (4.7)

This partitioning (or mesh) is then used as the basis for defining the functions used in the solution approximation. Spatially varying properties of the domain are herein only considered to have a piecewise constant variation across elements. This includes the material properties $D(r)$ and $\Sigma(r)$, the boundary condition terms and the prescribed fixed source $S(r)$.

The solution $\phi$ of equations (4.5) and (4.6), now called the full solution
\( \phi_{\text{full}} \), is decomposed into two components

\[
\phi_{\text{full}}(r) = \phi_{\text{cg}}(r) + \phi_{\text{sgs}}(r),
\]  

where \( \phi_{\text{cg}} \) represents a continuous globally resolved component and \( \phi_{\text{sgs}} \) represents the inner element discontinuous subgrid scale component. Note that in the research presented herein the subgrid scale component \( \phi_{\text{sgs}} \) will have discontinuities at element-element boundaries but remain continuous within each element. Also, the subgrid scale component is actually the sum of \( n_{\text{ele}} \) individual terms which are intended to provide a local enrichment to the full solution. The subgrid scale component can be considered to represent the error of the continuous global component. Therefore as resolution is increased to the continuous global component the value (and hence contribution to the full solution) of the subgrid scale component should tend to zero.

To form a well-posed problem the full solution decomposition is complemented with the boundary condition

\[
\phi_{\text{sgs}}(r) |_{\Gamma_{\text{ele}}} = 0 \quad \forall \text{iele},
\]  

where \( \Gamma_{\text{ele}} \) is the surface bounding the element \( \text{iele} \) but does not include inner element surfaces that are also part of the outer full domain surface. A crucial aspect of the method centres on how this inner element boundary condition is applied within the formulation. The enforcement of this boundary condition ensures that each inner element subgrid scale solution is independent of every other as no information is directly communicated between them.

The two components of the full solution are now approximated as a finite series expansion of known functions given by

\[
\phi_{\text{cg}}(r) \approx \tilde{\phi}_{\text{cg}}(r) = \sum_{i} N_i(r) \phi_{\text{cg}}^i,
\]

\[
\phi_{\text{sgs}}(r) \approx \tilde{\phi}_{\text{sgs}}(r) = \sum_{j} Q_j(r) \phi_{\text{sgs}}^j,
\]

where \( \phi_{\text{cg}}^i \) and \( \phi_{\text{sgs}}^j \) are the coefficients of expansion of the continuous global and subgrid scale components respectively. Therefore the approximate full
solution to the residual equation is given by

\[
\tilde{\phi}_{\text{full}}(r) = \tilde{\phi}_{\text{cg}}(r) + \tilde{\phi}_{\text{sgs}}(r),
\]

\[
= \sum_i N_i(r) \phi_{i\text{cg}} + \sum_j Q_j(r) \phi_{j\text{sgs}}.
\]

The functions \(N_i\) represent the set of linearly independent continuous basis functions defined to span the whole domain such as to conform to the mesh. Similarly, the functions \(Q_j\) represent the set of linearly independent discontinuous basis functions defined to span within each element as needed. A large degree of flexibility is available in the choice of the basis function sets \(N_i\) and \(Q_j\). As each inner element expansion is independent of all other inner elements the flexibility also exists to have different orders and even different families of basis functions used in the approximation of the sub grid scale component within the same problem. However, the method is initially only analysed in section 4.3 with the use of standard Lagrange finite element shape functions of polynomial order linear and quadratic with the same order used for each inner element expansion.

To determine the coefficients of the expansion approximation, hence obtain a solution, a standard Galerkin Weighted Residual method is used where the weight functions are the combined set of all \(N_i\) and \(Q_j\). Integrating the weight and the combined residual equations (4.5) and (4.6) over the whole domain gives the weak form

\[
\int_\Omega N_i \mathcal{R}(\tilde{\phi}_{\text{cg}}) d\Omega + \int_\Gamma N_i \mathcal{K}(\tilde{\phi}_{\text{cg}}) d\Gamma + \int_\Omega N_i \mathcal{R}(\tilde{\phi}_{\text{sgs}}) d\Omega + \int_\Gamma N_i \mathcal{K}(\tilde{\phi}_{\text{sgs}}) d\Gamma = 0,
\]

\[
\int_\Omega Q_j \mathcal{R}(\tilde{\phi}_{\text{cg}}) d\Omega + \int_\Gamma Q_j \mathcal{K}(\tilde{\phi}_{\text{cg}}) d\Gamma + \int_\Omega Q_j \mathcal{R}(\tilde{\phi}_{\text{sgs}}) d\Omega + \int_\Gamma Q_j \mathcal{K}(\tilde{\phi}_{\text{sgs}}) d\Gamma = 0,
\]

for all \(N_i\) and \(Q_j\). Note that it is the weighted residual of the full solution that is equal to zero, not the weighted residual of the continuous global and sub grid scale components individually. Moving the sources to the right hand side and written in matrix vector notation this becomes

\[
\begin{pmatrix}
A & B \\
C & D
\end{pmatrix}
\begin{pmatrix}
\tilde{\phi}_{\text{cg}} \\
\tilde{\phi}_{\text{sgs}}
\end{pmatrix} =
\begin{pmatrix}
S_{cg} \\
S_{sgs}
\end{pmatrix},
\]
where $\bar{\phi}_{cg}$ and $\bar{\phi}_{sgs}$ are the vectors of to be determined coefficients associated with the continuous global and sub grid scale components respectively. The right hand source vectors are given by

$$S_{cg} = \int_{\Omega} N_i S(r) d\Omega, \quad (4.17)$$

$$S_{sgs} = \int_{\Omega} Q_j S(r) d\Omega, \quad (4.18)$$

where $S(r)$ is a prescribed source which is taken as piecewise constant over an element. The individual sub matrices are given by

$$A_{ij} = \int_{\Omega} N_i \mathcal{L}(N_j) d\Omega + \int_{\Gamma} N_i K(N_j) d\Gamma, \quad (4.19)$$

$$B_{ij} = \int_{\Omega_{k_ele}} N_i \mathcal{L}(Q_j) d\Omega + \int_{\Gamma} N_i K(Q_j) d\Gamma, \quad (4.20)$$

$$C_{ij} = \int_{\Omega_{k_ele}} Q_i \mathcal{L}(N_j) d\Omega + \int_{\Gamma} Q_i K(N_j) d\Gamma, \quad (4.21)$$

$$D_{ij} = \int_{\Omega_{k_ele}} Q_i \mathcal{L}(Q_j) d\Omega + \int_{\Gamma} Q_i K(Q_j) d\Gamma, \quad (4.22)$$

where the integration associated with the sub matrices $B$, $C$ and $D$ need only be performed over the relevant element $k_{ele}$ within which the discontinuous shape functions are defined as they have zero value (hence zero derivative) every where else. The $A$ sub matrix can be seen to be identical to that which would arise from the application of the standard Continuous Galerkin method, without the decomposition of the full solution into two components. Following this standard method through to completion the volume diffusion term within $A$ is integrated by parts reducing the order of the derivatives present. The surface integrals arising from the integration by parts are negated with the boundary condition integrals where appropriate. The reflect boundary condition directly cancels this term and is a natural boundary condition. The vacuum boundary condition leaves a surface integral term that is implicitly included into $A$. The zero boundary condition is assumed automatically satisfied by the approximating solution and with the weight functions appropriately defined as zero on surfaces with this constraint. This implies that the surface integrals arising from the integration by parts with respect to surfaces that have a zero boundary condition are...
neglected. Therefore the final form of the sub matrix $A$ is given by

$$A_{ij} = \int_{\Omega} \nabla N_i \cdot D(r) \nabla N_j d\Omega + \int_{\Gamma_V} 0.5N_iN_j d\Gamma + \int_{\Omega} \Sigma(r) N_iN_j d\Omega. \quad (4.23)$$

The sub matrices $B$, $C$ and $D$ follow a similar argument to that given for $A$ above when the weight and basis function associated with the specific integrals of each have a non zero value on the outer surface of the full domain. This implies the correct application of the problem boundary condition to the full solution as it is enforced on both the continuous global and sub grid scale components. When the weight and basis functions are zero on the outer full domain surface (the homogeneous functions) then a different formulation with respect to the diffusion term is utilised for the sub matrices $B$, $C$ and $D$ as follows.

4.2.2.1. Formulation of the Sub Matrix $D$

First consider the diffusion term $D_{diff}$ of the sub matrix $D$ given by

$$D_{diff} \bar{\phi}_{sgs} = -D_{kele} \int_{\Omega_{kele}} Q_i \nabla \cdot \nabla \bar{\phi}_{sgs} d\Omega \quad \forall Q_i, \quad (4.24)$$

where $D_{kele}$ is the piecewise constant variation of the isotropic diffusion coefficient on element $kele$ over which $Q_i$ is only non zero. The vector of auxiliary functions $J_{sgs}$ is introduced as

$$J_{sgs} = \nabla \phi_{sgs}. \quad (4.25)$$

The components of $J_{sgs}$ for each spatial direction $k$ are given by

$$J_{sgsk} = \frac{\partial \phi_{sgs}}{\partial x_k}, \quad (4.26)$$

where $x_k$ is the spatial variable in the $k$ direction. Approximating both the sub grid scale solution variable and auxiliary functions with the same basis set expansion gives

$$\sum_j Q_j(r) J_{sgsk}^j \approx \sum_j \frac{\partial Q_j(r)}{\partial x_k} \phi_{sgs}^j, \quad (4.27)$$
where \( J_{s gs}^k \) and \( \phi_{s gs}^j \) are the coefficients of each expansion. Assuming that the coefficients of the solution variable were known then the coefficients of the auxiliary function can be determined via a Galerkin Projection using the \( Q_i \) basis set as weights. This is expressed as

\[
\int_{\Omega_{kele}} Q_i \sum_j Q_j J_{s gs}^j d\Omega = \int_{\Omega_{kele}} Q_i \sum_j \frac{\partial Q_j(r)}{\partial x_k} \phi_{s gs}^j d\Omega \quad \forall \ Q_i. \quad (4.28)
\]

Integrating the volume integral of the gradient of the solution variable on the right hand side by parts gives

\[
\int_{\Omega_{kele}} Q_i \sum_j Q_j J_{s gs}^j d\Omega = -\int_{\Omega_{kele}} \frac{\partial Q_i(r)}{\partial x_k} \sum_j Q_j \phi_{s gs}^j d\Omega
+ \int_{\Gamma_{kele}} Q_i \sum_j Q_j \phi_{s gs}^j n_k d\Gamma \quad \forall \ Q_i, \quad (4.29)
\]

where \( n_k \) is the component of the outward unit normal vector in the \( k \) spatial direction of the element bounding surface \( \Gamma_{kele} \). Applying the inner element boundary condition (4.9) implies that the surface integral term vanishes. This method corresponds to a weak enforcement of the zero Dirichlet boundary condition. However, as discussed in subsection 4.2.4 this is not the only method to treat this surface integral and apply the inner element boundary condition.

Using matrix vector notation to represent equation (4.29) gives

\[
MQQ \tilde{J}_{s gs} = GQQ \tilde{\phi}_{s gs}, \quad (4.30)
\]

where \( \tilde{J}_{s gs} \) and \( \tilde{\phi}_{s gs} \) are the vectors of coefficients associated with the auxiliary and solution variable respectively. The matrices \( MQQ \) and \( GQQ \) which are block element wise are given by

\[
MQQ_{ij} = \int_{\Omega_{kele}} Q_i Q_j d\Omega, \quad (4.31)
\]

\[
GQQ_{ij} = -\int_{\Omega_{kele}} \frac{\partial Q_i(r)}{\partial x_k} Q_j d\Omega. \quad (4.32)
\]

The matrix \( MQQ \) is an element mass matrix and the matrix \( GQQ \) is an element advective matrix in the \( k \) spatial direction. The auxiliary function vector of coefficients for each direction can then be found via inversion of
the element mass matrix such that

\[ J_{sgs_k} = M_{QQ}^{-1} G_{QQ_k} \tilde{\phi}_{sgs}. \] (4.33)

Using the definition of the auxiliary function (4.25) and the approximate expansion (4.27) the diffusion term (4.24) becomes

\[ D_{diff} \tilde{\phi}_{sgs} = -D_{kele} \int_{\Omega_{kele}} \sum_k \sum_j \left( Q_i \frac{\partial Q_j(r)}{\partial x_k} J_{sgs_k}^j \right) d\Omega \quad \forall Q_i. \] (4.34)

On inspection of this equation with the definition of \( G_{QQ} \) the diffusion contribution to the sub matrix \( D \) for the element \( kele \) is given by

\[ D_{diff} = D_{kele} \sum_k \left( G_{QQ_k}^T M_{QQ}^{-1} G_{QQ_k} \right). \] (4.35)

Therefore the final form of the sub matrix \( D \) for the homogeneous weight and basis functions is given by

\[ D_{ij} = D_{kele} \sum_k \left( G_{QQ_k}^T M_{QQ}^{-1} G_{QQ_k} \right) + \int_\Omega \Sigma(r) Q_i Q_j d\Omega, \] (4.36)

where the \( Q_i \) and \( Q_J \) are defined as only non zero within the element \( kele \).

### 4.2.2.2. Formulation of the Sub Matrix \( B \)

Now consider the diffusion term \( B_{diff} \) of the sub matrix \( B \) given by

\[ B_{diff} \tilde{\phi}_{sgs} = \sum_{kele} \left( -D_{kele} \int_{\Omega_{kele}} N_i \nabla \cdot \nabla \tilde{\phi}_{sgs} d\Omega \right) \quad \forall N_i. \] (4.37)

The method is very similar to that used for \( D_{diff} \) with differences arising due to the presence of continuous weight functions \( N_i \) and the desire to produce a formulation such that the large matrix formed from the sub matrices \( A \), \( B \), \( C \) and \( D \) is still symmetric. The latter point implies that a formulation with \( B = C^T \) is necessary.
Integrating equation (4.37) by parts gives

\[ B_{\text{diff}} \bar{\phi}_{\text{sgs}} = \sum_{\text{kele}} D_{\text{kele}} \left( \int_{\Omega_{\text{kele}}} \nabla N_i \cdot \nabla \tilde{\phi}_{\text{sgs}} d\Omega - \int_{\Gamma_{\text{kele}}} N_i n \cdot \nabla \tilde{\phi}_{\text{sgs}} d\Gamma \right) \quad \forall N_i. \quad (4.38) \]

Through consideration of conservation of the full neutron flux solution \( \phi_{\text{full}} \) it can be stated that

\[ \sum_{\text{kele}} D_{\text{kele}} \left( \int_{\Gamma_{\text{kele}}} n \cdot \nabla \phi_{\text{full}} d\Gamma \right) \equiv 0, \quad (4.40) \]

where \( \Gamma_{\text{kele}} \) are the inner element surfaces that do not coincide with the outer boundary of the full domain. This basically states that the neutron current out of one volume element across a particular surface equals the neutron current into the neighbouring element connected by the particular surface. Considering the full solution decomposition and that the continuous global solution component \( \phi_{\text{cg}} \) implicitly satisfies

\[ \sum_{\text{kele}} D_{\text{kele}} \left( \int_{\Gamma_{\text{kele}}} n \cdot \nabla \phi_{\text{cg}} d\Gamma \right) \equiv 0, \quad (4.41) \]

this implies that

\[ \sum_{\text{kele}} D_{\text{kele}} \left( \int_{\Gamma_{\text{kele}}} n \cdot \nabla \phi_{\text{sgs}} d\Gamma \right) \equiv 0. \quad (4.42) \]

As the weight function \( N_i \) is continuous across element-element boundaries it can now be stated that

\[ \sum_{\text{kele}} D_{\text{kele}} \left( \int_{\Gamma_{\text{kele}}} N_i n \cdot \nabla \phi_{\text{sgs}} d\Gamma \right) \equiv 0 \quad \forall N_i. \quad (4.43) \]

This implies that the diffusion term \( B_{\text{diff}} \) reduces to

\[ B_{\text{diff}} \bar{\phi}_{\text{sgs}} = \sum_{\text{kele}} D_{\text{kele}} \left( \int_{\Omega_{\text{kele}}} \nabla N_i \cdot \nabla \tilde{\phi}_{\text{sgs}} d\Omega \right) \quad \forall N_i. \quad (4.44) \]

As with \( D_{\text{diff}} \) a vector of auxiliary functions is introduced and the formu-
lution from equation (4.25) to equation (4.33) is used such that

\[ B_{\text{diff}} = D_{\text{kele}} \sum_k \left( G_{\text{NQ}k} M^{-1}_{\text{QQ}} G_{\text{QQ}k} \right), \]  

(4.45)

where the \( G_{\text{NQ}k} \) term is given by

\[ G_{\text{NQ}kij} = -\int_{\Omega_{\text{kele}}} \frac{\partial N_i(r)}{\partial x_k} Q_j d\Omega. \]

(4.46)

Note that this term differs from that given by Candy (2008) where both the \( G \) terms and the mass matrix \( M \) were formed from cross space basis functions. The method derived here is chosen such that the mass matrix remains square and with a unique inverse.

Therefore the final form of the sub matrix \( B \) for the homogeneous weight and basis functions is given by

\[ B_{ij} = D_{\text{kele}} \sum_k \left( G_{\text{NQ}k,ir} M^{-1}_{\text{QQ},rs} G_{\text{QQ}k,sj} \right) + \int_{\Omega} \Sigma(r) N_i Q_j d\Omega, \]

(4.47)

where the \( Q_j \) are defined as only non zero within the element \( \text{kele} \).

4.2.2.3. Formulation of the Sub Matrix \( C \)

Finally consider the diffusion term \( C_{\text{diff}} \) of the sub matrix \( C \) given by

\[ C_{\text{diff}} \bar{\phi}_{\text{sgs}} = \sum_{\text{kele}} \left( -D_{\text{kele}} \int_{\Omega_{\text{kele}}} Q_i \nabla \cdot \nabla \bar{\phi}_{\text{cg}} d\Omega \right) \quad \forall Q_i. \]

(4.48)

Unlike the formulation for \( B_{\text{diff}} \) there is no integration by parts here. This is because the inner surface integrals that would appear would not cancel due to the discontinuous weight function. Similar to before a vector of auxiliary functions \( J_{\text{cg}} \) is introduced as

\[ J_{\text{cg}} = \nabla \phi_{\text{cg}}. \]

(4.49)

The components of \( J_{\text{cg}} \) for each spatial direction \( k \) are given by

\[ J_{\text{cgk}} = \frac{\partial \phi_{\text{cg}}}{\partial x_k}, \]

(4.50)
where \( x_k \) is the spatial variable in the \( k \) direction. To generate a formulation where \( B = C^T \) the solution variable \( \phi_{cg} \) is approximated with an expansion of \( N_j \) and the vector of auxiliary functions approximated with an expansion of \( Q_j \) such that

\[
\sum_j Q_j(r)J^j_{cgk} \approx \sum_j \frac{\partial N_j(r)}{\partial x_k} \phi^j_{cg},
\]

where \( J^k_{cg} \) and \( \phi^j_{cg} \) are the coefficients of each expansion. Assuming that the coefficients of the solution variable were known then the coefficients of the auxiliary function can be determined via a Galerkin Projection using the \( Q_i \) basis set as weights. This is expressed as

\[
\int_{\Omega_{kele}} Q_i \sum_j Q_j J^j_{cgk} d\Omega = \int_{\Omega_{kele}} Q_i \sum_j \frac{\partial N_j(r)}{\partial x_k} \phi^j_{cg} d\Omega \quad \forall Q_i. \tag{4.52}
\]

As there is no inner surface constraint for the continuous global solution variable \( \phi_{cg} \) the volume integral on the right hand side is not integrated by parts. Expressing this relation in matrix vector notation gives

\[
M_{QQ} \tilde{J}_{cgk} = G^T_{QN} \tilde{\phi}_{cg}, \tag{4.53}
\]

where \( \tilde{J}_{cgk} \) and \( \tilde{\phi}_{cg} \) are the vectors of coefficients associated with the auxiliary and solution variable respectively. Also, the definition of the matrices \( M \) and \( G \) follow from the previous definitions given by equations (4.31) and (4.32). Via inversion of the square element wise mass matrix the coefficients of the vector of auxiliary functions expansion are found as

\[
\tilde{J}_{cgk} = M^{-1}_{QQ} G^T_{QN} \tilde{\phi}_{cg}. \tag{4.54}
\]

Using this result the diffusion term \( C_{diff} \) is found to be

\[
C_{diff} = D_{kele} \sum_k \left( G^T_{QQk} M^{-1}_{QQ} G^T_{NNk} \right). \tag{4.55}
\]

Therefore the final form of the sub matrix \( C \) for the homogeneous weight
and basis functions is given by

\[ C_{ij} = D_{kele} \sum_k \left( G_{QQ_{ks}}^T M_{QQ_{rs}}^{-1} G_{NN_{ks}}^T \right) + \int_{\Omega} \Sigma(r) Q_i N_j d\Omega, \tag{4.56} \]

where the \( Q_i \) are defined as only non zero within the element \( kele \). On inspection of equation (4.47) and (4.56) it is easily observed that \( B = C^T \) as desired within the formulation. Interestingly via numerical observation it was discovered that the terms \( B_{diff} \) and \( C_{diff} \) on regular Cartesian aligned meshes (i.e. slab geometry, structured quadrilateral XY geometry and structured hexahedral XYZ geometry) using linear and quadratic Lagrange basis functions were actually zero. This was not found to hold on more irregular meshes.

### 4.2.3. Full Domain Outer Surface Boundary Condition

**Simplification**

The previous section described how the full outer domain boundary conditions should be implemented to both the continuous global inner element sub grid scale components. However, to simplify the computational implementation of the formulation an approximation to this is now given. All the results herein use this approximation. Motivated by the results of Candy (2008) and Buchan et al. (2010) and primarily due to the formulation it is to be expected that the sub grid scale component of the full solution will consist of a small variation (or correction) in comparison to the continuous global component. To simplify the application of the outer domain surface boundary condition rather than apply as needed the reflect and vacuum where appropriate the inner element weak zero boundary condition was applied everywhere instead. The correct outer boundary condition is still applied to the continuous global component as needed in an identical manner as would done for a conventional Continuous Galerkin formulation. Therefore consistency will be maintained for the outer domain surfaces that have a zero Dirichlet condition but not for the vacuum and reflect conditions. This will considered when presenting the numerical examples in section 4.3. This approximation was numerically implemented first. Then the method to apply the correct outer boundary conditions was attempted numerically however it failed to produce anything sensible. It was not deduced as to
whether this was due to the formulation or an incorrect implementation of the formulation.

4.2.4. Inner Element Surface Integral Treatment

Subtle variations in the formulation of the application of the inner surface boundary condition give rise to slightly different sub grid scale methods that have different stability and accuracy characteristics. In the original method presented in subsection 4.2.2 the inner surface weak zero boundary condition is applied in the formulation of the $B$ and $D$ sub matrices. Recalling this the introduction of a vector of auxiliary functions resulted in the equation

$$
\int_{\Omega_{kele}} Q_i \sum_j Q_j J_{sgs} d\Omega = - \int_{\Omega_{kele}} \frac{\partial Q_i(r)}{\partial x_k} \sum_j Q_j \phi^j_{sgs} d\Omega + \int_{\Gamma_{kele}} Q_i \sum_j Q_j \phi^j_{sgs} n_k d\Gamma \quad \forall Q_i. \quad (4.57)
$$

The original method stated that as the sub grid scale component is to be set to zero on inner surface elements then the surface integral in equation (4.57) vanishes. However, as will be shown in the numerical examples section this original method was found to be unstable or worse unsolvable under certain problem conditions. For example any problem with a material region which resulted in no absorption coefficient in the matrix assembly generated a $D$ sub matrix that was singular. This was independently verified by Pain (2010) for 1D problems so as to have increased confidence that this was not an computational implementation error. Also a 2D XY geometry 2 energy group whole nuclear core benchmark characteristic of a BWR was found to have a solution that diverged after having converged to a degree of accuracy of $1.0E^{-4}$ with respect to the eigenvector.

The simplest solution to problems involving materials that generated a zero absorption coefficient was to introduce an artificial one into the $D$ sub matrix alone. This would modify the original method such that the $D$ sub matrix is given by

$$
D_{ij} = D_{kele} \sum_k \left( G^T_{QQ_{krr}} M^{-1}_{QQ_{rs}} G_{QQ_{sjsj}} \right) + \int_{\Omega} \max(\alpha, \Sigma(r)) Q_i Q_j d\Omega,
$$

(4.58)
where $\alpha$ is a problem dependent stabilisation factor. Note that setting $\alpha$ to infinity (or an effectively large number) would force the sub grid scale component solution to zero and that setting $\alpha$ to zero would recover the original method. The use of a tunable problem dependent parameter is an undesirable method but will be considered in the numerical examples section for the cases that required it using the original method.

An alternative suggestion is to treat the surface integral in equation (4.57) differently, in a similar way as different Discontinuous Galerkin methods treat surface integrals with respect to the diffusion term. It is recognised that the the sub grid scale solution on each element inner surface has a discontinuity. There is the solution value (to be determined) and the weakly enforced inner element zero boundary condition. The original method always takes the zero for this term. However the inner surface solution value could be taken as the interpolated value

$$\phi_{sgs_{\Gamma_{ele}}} = \alpha \phi_{sgs} + (1 - \alpha) \phi_{sgs_{BC}}, \quad (4.59)$$

where $\phi_{sgs_{BC}}$ is zero and $\phi_{sgs}$ the value to be determined. Then equation (4.57) would be implemented as

$$\int_{\Omega_{ele}} Q_i \sum_j Q_j J_{sGs k} d\Omega = - \int_{\Omega_{ele}} \frac{\partial Q_i(r)}{\partial x_k} \sum_j Q_j \phi_{sGs} d\Omega$$

$$+ \int_{\Gamma_{ele}} \alpha Q_i \sum_j Q_j \phi_{sGs} n_k d\Gamma \quad \forall \ Q_i, \quad (4.60)$$

with a surface term remaining. Using this new relationship the $D_{diff}$ term could be written as

$$D_{diff} = D_{kele} \sum_k \left( G_{QQ}^T M_{QQ}^{-1} (G_{QQ} + H_{QQ}) \right), \quad (4.61)$$

where

$$H_{QQ_{kij}} = \int_{\Gamma_{ele}} \alpha Q_i \sum_j Q_j \phi_{sGs} n_k d\Gamma \quad \forall \ Q_i. \quad (4.62)$$

However implementation of this produced non sensible results. A method that did produce more sensible stable results is if the $D_{diff}$ term was given.
\[ D_{\text{diff}} = D_{\text{kiele}} \sum_k \left( G^{*T}_{QQk} M^{-1}_{QQ} G^*_k \right), \] (4.63)

where

\[ G^{*}_{QQk} = G_{QQk} + H_{QQk}. \] (4.64)

If the \( \alpha \) term is set to 0.5 this is characteristic of the Bassi Rebay Discontinuous method for the approximation of the surface variable and if the \( \alpha \) term is set to 0 then the original method is recovered. Note that this change to the inner element surface treatment is considered for the \( D \) sub matrix and not for the \( B \) sub matrix as it is not inverted. Also, if this treatment was applied to the \( B \) sub matrix it is not obvious if a corresponding treatment should (or could) be applied to the \( C \) sub matrix such that \( B = C^T \) will be maintained. Although this suggested method is characteristic of the Bassi Rebay Discontinuous method it differs in that only an approximation of the solution variable is needed. A corresponding approximation of the auxiliary functions on the inner surfaces is not needed in the sub grid scale formulation presented. Although the \textit{ad-hoc} derivation suggests it is actually included. Note that this is not the case with the DG method where the method is derived more rigorously.

Another suggestion is to use a form of Modified Local Discontinuous Galerkin method for the treatment of the diffusion term. This formulates the \( D_{\text{diff}} \) term as

\[ D_{\text{diff}} = D_{\text{kiele}0.5} \sum_k \left( G^{+T}_{QQk} M^{-1}_{QQ} G^+G^+_{QQk} + (-G^{-T}_{QQk}) M^{-1}_{QQ} (-G^{-}_{QQk}) \right), \] (4.65)
where the directional components of the vectors $G^{+}_{QQ}$ and $G^{-}_{QQ}$ are given as

$$G^{+}_{QQ_{ij}} = -\int_{\Omega_{kcel}} \frac{\partial Q_i(r)}{\partial x_k} \sum_j Q_j \phi^{j}_{sgs} d\Omega$$

$$+ \int_{\Gamma_{kelnk>0}} \alpha Q_i \sum_j Q_j \phi^{j}_{sgs} n_k d\Gamma \quad \forall Q_i, \quad (4.66)$$

$$G^{-}_{QQ_{ij}} = +\int_{\Omega_{kcel}} \frac{\partial Q_i(r)}{\partial x_k} \sum_j Q_j \phi^{j}_{sgs} d\Omega$$

$$- \int_{\Gamma_{kelnk<0}} \alpha Q_i \sum_j Q_j \phi^{j}_{sgs} n_k d\Gamma \quad \forall Q_i. \quad (4.67)$$

The $\alpha$ parameter is chosen to be 1 and if set to 0 the original method is recovered. As before this method of treating the diffusion term is applied to the $D$ sub matrix but not the $B$ sub matrix for the same reasons discussed.

The following naming convention is now used herein to distinguish between the different methods:

1. $SGSO$ refers to the original method,

2. $SGSOMin$ refers to the original method with a minimum absorption parameter introduced,

3. $SGSBR$ refers to the method with the Bassi Rebay characteristic surface integrals for the diffusion term of $D$,

4. $SGSMLDG$ refers to the method which treats the diffusion term in $D$ with a Modified Local Discontinuous Galerkin method.

### 4.2.5. Static Condensation Solution Algorithm

Recalling the matrix vector representation resulting from the full solution decomposition and the use of the Galerkin Residual Method as

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix} \begin{pmatrix} \bar{\phi}_{cg} \\ \bar{\phi}_{sgs} \end{pmatrix} = \begin{pmatrix} S_{cg} \\ S_{sgs} \end{pmatrix}, \quad (4.68)$$

where $\bar{\phi}_{cg}$ and $\bar{\phi}_{sgs}$ are the vectors of to be determined coefficients associated with the continuous global and sub grid scale components respectively.
Explicitly expanding this out gives

\[ A\bar{\phi}_{cg} + B\bar{\phi}_{sgs} = S_{cg}, \]  
\[ C\bar{\phi}_{cg} + D\bar{\phi}_{sgs} = S_{sgs}. \]

(4.69)  
(4.70)

Rearranging equation (4.70) gives

\[ \bar{\phi}_{sgs} = D^{-1}(S_{sgs} - C\bar{\phi}_{cg}). \]  
(4.71)

Substitution of equation (4.71) into equation (4.69) with rearrangement gives

\[ (A - BD^{-1}C)\bar{\phi}_{cg} = S_{cg} - BD^{-1}S_{sgs}. \]

(4.72)

This process is commonly referred to as static condensation as the continuous global component can now be found through the manipulation of the matrices involved with the sub grid scale formulation. After the continuous global component is found the sub grid scale component can be found and then the full solution recovered. Due to the discontinuous basis functions the sub matrices B, C and D are all element wise block diagonal. They can therefore be constructed and used element by element in the formation of the continuous linear system to solve for. The element wise diagonal blocks of the sub matrix D can be inverted via a direct method such as Cholesky Factorisation. The matrix \( A - BD^{-1}C \) that is to solved within an iterative solver has the same sparsity pattern as the matrix A. Therefore no extra work is required to solve the continuous global solution in comparison to standard Continuous Galerkin methods. Extra work is required in the assembly, inversion and multiplication of the element wise sub matrices B, C and D. As the A matrix is usually stored in computational memory as it is solved then it is advocated that the matrices \( D^{-1}, BD^{-1} \) and \( D^{-1}C \) (which are formed when A is formed) are also stored as they are used in forming the source and finding the sub grid scale component solution.

4.2.6. Extension to Multigroup Neutron Diffusion, Eigenvalue and Time Dependent Problems

The extension of the sub grid scale formulation to multigroup fixed source, eigenvalue and time dependent problems is shown. The multigroup fixed
source problem is defined as (with the spatial variable $r$ omitted)

$$
- \nabla \cdot D_g \nabla \phi_{full_g} + \Sigma_{r_g} \phi_{full_g} = S_{fix_g} + \sum_{g' = 1}^{G} \Sigma_{s_{g' \rightarrow g}} \phi_{full_{g'}} + (1 - \beta) \chi_{pg} \sum_{g' = 1}^{G} \nu_{g'} \Sigma_{f_{g'}} \phi_{full_{g'}} + \sum_{l} \chi_{dg}^l \lambda^l C^l \quad \forall \ r \in \Omega, \quad (4.73)
$$

where standard notation is used.

The discretised within group neutron diffusion equation is then given by equation (4.68) with the source terms now taking the form

$$
S_{cg_i} = \int_{\Omega} N_i S_{fix_g} d\Omega + \int_{\Omega} \sum_{g' = 1}^{G} \Sigma_{s_{g' \rightarrow g}} N_i \sum_{j} N_j \phi_{cg_{g'}}^j d\Omega
$$

$$
+ \int_{\Omega} \sum_{g' = 1}^{G} \Sigma_{s_{g' \rightarrow g}} N_i \sum_{j} Q_j \phi_{sgs_{g'}}^j d\Omega + \int_{\Omega} (1 - \beta) \chi_{pg} \sum_{g' = 1}^{G} \nu_{g'} \Sigma_{f_{g'}} N_i \sum_{j} N_j \phi_{cg_{g'}}^j d\Omega
$$

$$
+ \int_{\Omega} (1 - \beta) \chi_{pg} \sum_{g' = 1}^{G} \nu_{g'} \Sigma_{f_{g'}} N_i \sum_{j} Q_j \phi_{sgs_{g'}}^j d\Omega + \int_{\Omega} \sum_{l} \chi_{dg}^l \lambda^l N_i C^l, \quad (4.74)
$$

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\[ S_{sgs_i} = \int_{\Omega} Q_i S_{fix_g} d\Omega \]

\[ + \int_{\Omega} \sum_{g' = 1}^{G} \sum_{g' \neq g} \Sigma_{sg' \rightarrow g} Q_i \sum_{j} N_j \phi_{cag'}^j d\Omega \]

\[ + \int_{\Omega} \sum_{g' = 1}^{G} \Sigma_{sg' \rightarrow g} Q_i \sum_{j} Q_j \phi_{sgs,g'}^j d\Omega \]

\[ + \int_{\Omega} (1 - \beta) \chi_{pg} \sum_{g' = 1}^{G} \nu_{g'} \Sigma_{f_g} Q_i \sum_{j} N_j \phi_{cag'}^j d\Omega \]

\[ + \int_{\Omega} (1 - \beta) \chi_{pg} \sum_{g' = 1}^{G} \nu_{g'} \Sigma_{f_g} Q_i \sum_{j} Q_j \phi_{sNS,g'}^j d\Omega \]

\[ + \int_{\Omega} \sum_{l} \chi_{dg}^l \lambda^l Q_i C^l, \quad (4.75) \]

The multigroup fixed source problem can then be solved as standard via a block Gauss Seidel algorithm that sweeps the within energy group equations updating the source vector as needed. With the extension to multigroup fixed source problems the further extension to eigenvalue and time dependent problems follows. This is because the fixed source solution forms the basis of the iterative schemes conventionally used in the solution of the eigenvalue and time dependent problem.

### 4.3. Sub Grid Scale Numerical Examples

In this section the SGS methods formulated in section 4.2 are applied and analysed for a range of test cases. Test cases are initially extremely simple and then increase in complexity. Eigenvalue problems are considered in 1D and 2d with either one or two energy groups. Only problems that have structured meshes are considered. Solutions where appropriate are compared to the fine mesh CG solution that is taken as the exact. All test cases were constructed in the continuous Quality Assurance infrastructure described in chapter 3.

All macroscopic cross sections are given in units of \( cm^{-1} \). Unless stated
it should be assumed that the isotropic transport cross section is given by

\[ \Sigma_{tr_g} = \Sigma_{tg} \]  \hspace{1cm} (4.76)

and that the isotropic diffusion coefficient used is given by

\[ D_g = \frac{1}{3\Sigma_{tr_g}}. \]  \hspace{1cm} (4.77)

Tests cases all use Lagrange family shape functions of polynomial order linear (l) or quadratic (q). Possible permutations of the shape function order for the SGS method analysed are l-l, l-q, q-l and q-q. The first letter in this notation refers to the continuous global component and the second letter the sub grid scale component. The relative \( K_{eff} \) error, which is used to give a global error estimate, is given by

\[ \frac{K_{eff_{exact}} - K_{eff}}{K_{eff_{exact}}}. \]  \hspace{1cm} (4.78)

Errors are compared for order of convergence where the order is deduced via comparison of gradients with functions given by

\[ f(x) = kx^{-N}, \]  \hspace{1cm} (4.79)

where \( k \) is an arbitrary constant taken as 1.0 and \( N \) is the integer being the order of convergence.

Results presented in graphs use linear interpolation through the data points unless stated. For the visualisation of the full solution if the basis set of the continuous global and sub grid scale component expansions are of the same order then the full solution is represented by the discontinuous basis set of the same order. The coefficients of the expansion of the full solution are obtained in this case via a simple summation of the two components. If the basis set of the continuous global and sub grid scale component expansions have a different order then the component with the lower order is Galerkin Projected to a discontinuous basis set of the higher order. The full solution is then found via simple summation as before. For example, for a l-q SGSO solution the l CG component is Galerkin Projected to a q
discontinuous basis set via

\[ \bar{\phi}_{cg}^{GP} = M_{QQ}^{-1} M_{QN} \bar{\phi}_{cg}, \quad (4.80) \]

where

\[ M_{QQ_{ij}} = \int_{\Omega_{el}} Q_i Q_j d\Omega, \quad (4.81) \]
\[ M_{QN_{ij}} = \int_{\Omega_{el}} Q_i N_j d\Omega. \quad (4.82) \]

The \( \bar{\phi}_{cg}^{GP} \) and \( \bar{\phi}_{cg} \) are the vectors of coefficients associated with the expansion of the Galerkin Projected CG component and the CG component respectively. The \( M \) are element wise mass matrices where the \( Q \) and \( N \) subscripts signify the discontinuous and continuous basis sets respectively. The full solution which is output for this example is given by

\[ \phi_{full} = \phi_{cg}^{GP} + \phi_{sgs}. \quad (4.83) \]

As the visualisation programs used require all fields to have the same mesh the Galerkin Projected component is also output rather than the original component. Therefore in the example discussed the field \( \phi_{cg}^{GP} \) is visualised rather than \( \phi_{cg} \). The Galerkin Projection will preserve the integral of the solution over the element but will not necessarily preserve point values. Note that this happens only for the spatial visualisation of the full solution and has no effect on the actual SGS formulation. Any element wise integrals of solutions (which can include power densities) are calculated and visualised exactly in the sense that no extra approximation is needed (the correct basis functions for each component are used). Also any quadratic spatial result is visualised via a linear interpolation through the quadratic nodal values as this is all that is available.

The use of certain methods for certain test cases produced results that are referred to as non sensible. This is used to signify that a very unrealistic solution was obtained where it is obvious that the numerical algorithm has failed, or literally did fail as an infinity of NaN resulted.
4.3.1. Homogeneous Infinite Square One Energy Group Eigenvalue

This test case is purposefully chosen to be extremely simple. It consists of one energy group, one homogeneous material within an infinite domain. This test case is problem 1 defined in the criticality benchmark set Sood et al. (2003). The discretised domain is modelled in 2D with structured quadrilateral mesh partitions. The outer domain boundary then has a reflective condition applied. The quadrilateral mesh is tested with all permutations possible being l-l, l-q, q-l and q-q. The material properties are given in table 4.1. The exact analytic Keff for this problem is given by

\[ K_{eff} = \frac{\nu \Sigma_f}{\Sigma_a} = 2.29032. \]  

(4.84)

All the SGS methods with the variations discussed above obtain this value to the accuracy of computational error (of the order of \(1.0E-12\)). The sub grid scale flux component in all cases was practically zero (of the order of \(1.0E-9\)). This important first test case shows that as expected the sub grid scale component is zero if there is sufficient accuracy in the continuous global component to resolve the solution. It also shows that the use of a reflective boundary condition which does not explicitly get applied to the sub grid scale component caused no issues.

<table>
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<th>Group</th>
<th>(\Sigma_t)</th>
<th>(\nu \Sigma_f)</th>
<th>(\Sigma_s)</th>
<th>(\Sigma_a)</th>
</tr>
</thead>
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<tr>
<td>1</td>
<td>0.32640</td>
<td>0.231744</td>
<td>0.225216</td>
<td>0.101184</td>
</tr>
</tbody>
</table>

Table 4.1.: Material properties of the test case Homogeneous Infinite Square One Energy Group Eigenvalue.

4.3.2. Homogeneous Finite Slab One Energy Group Eigenvalue

This test case consists of one energy group, one homogeneous material within a finite slab domain of length 4.513502 with vacuum boundary conditions on either side. Models are generated in 1D for the whole domain, in 1D with half the domain using a reflective condition and in 2D using a reflective condition on two opposing sides of a square domain which is meshed with
a regular quadrilateral grid to mirror the 1D case. These geometric models are illustrated in figure 4.1. The material property for this test case are identical to the test case Homogeneous Infinite Square One Energy Group Eigenvalue test case which are given in table 4.1. This test case is problem 6 in the criticality benchmark set Sood et al. (2003).

The difference between the 1D whole domain case and 1D half domain using a reflective boundary condition with respect to the $K_{eff}$ was found to be negligible (of the order $1.0E - 8$). This shows that the use of a reflective boundary condition which does not explicitly get applied to the sub grid scale component caused no issues in 1D. For the 1D whole domain
model the $K_{eff}$ with element mesh resolution is shown for the cases $l$ CG, $q$ CG, $l$-l SGO and $l$-q SGO in figure 4.2. Each method shown here converges from below. Figure 4.3 shows the corresponding relative $K_{eff}$ error for these cases with element mesh resolution. The $l$ CG and $l$-l SGO both show a second order convergence rate with respect to the number of elements although the $l$-l SGO method clearly offers an improvement in global solution accuracy compared to the $l$ CG method. For example for the case with 8 elements the relative $K_{eff}$ error for $l$ CG is $0.254\%$ and for $l$-l SGO is $0.073\%$. This corresponds to around a 70% reduction in this error measure. To converge the $K_{eff}$ to have a relative error of around 1pcm the $l$ CG method required about 128 elements (relative $K_{eff}$ error of $0.99pcm$). To achieve this convergence for the $l$-l SGO required around 64 elements (relative error of $1.16pcm$). With respect to the element mesh resolution the $q$ CG and $l$-q SGO show a third order convergence with the $l$-q SGO
Figure 4.3.: The relative $K_{eff}$ error versus number of elements for the test case *Homogeneous Finite Slab One Energy Group Eigenvalue* for the cases l CG, q CG, l-l SGSO and l-q SGSO.
Figure 4.4.: The relative $\text{Keff}$ error versus number of degrees of freedom into the solver for the test case *Homogeneous Finite Slab One Energy Group Eigenvalue* for the cases $q\text{ CG}$ and $1-q\text{ SGSO}$. 
Figure 4.5: Flux solution for the test case *Homogeneous Finite Slab One Energy Group Eigenvalue* for l-l SGSO method using 8 elements. The two scale components as well as the full solution are shown in comparison to the *exact* solution.

being the less accurate of the two. Figure 4.4 shows the relative Keff error for these two cases with number of unknowns into the solver (being the number of unknowns associated with the continuous global component in the SGS method). From this perspective the q CG and l-q SGSO have a fourth order convergence with the l-q SGSO being more accurate. Note that practically no difference was found between the use of implementation of q-q SGSO and l-q SGSO for this case.

Figure 4.5 shows the flux solution for the l-l SGSO method using 8 elements. The flux solution in each case is normalised to one unit integral flux. The two scale components and the full flux solution are shown with the *exact* for comparison. The sub grid scale component constitutes about 10% of the full solution at most located at the domain boundaries. The full solution for this method is piecewise constant within an element. Figure
Figure 4.6: Zoomed in flux solution for the test case *Homogeneous Finite Slab One Energy Group Eigenvalue* for l-l SGSO method using 8 elements. The 8 mesh l CG and *exact* solution are shown for comparison.
4.6 shows a close up of this flux solution within the middle of the domain problem. The 8 element 1 CG solution is also shown for comparison. The CG component of the l-l SGSO result can be observed to be highly node wise accurate. At the centre of the domain the relative difference between the CG component flux and the exact flux is 0.042%. In comparison the relative difference between the 1 CG flux and the exact flux is 0.42%. Due to the full solution of the SGSO method being element wise constant a point flux comparison with the standard CG method is not appropriate. Only a volume integral comparison is possible which has been previously shown using the Keff (which represents a whole domain volume integral).

The convergence of the Keff for the different SGS methods is compared in figures 4.7 and 4.8 respectively. Firstly it was observed that the l-q SGSBR method produced no sensible result (the Keff actually resembled that of
Figure 4.8: The relative $\text{Keff}$ error versus number of elements for the test case *Homogeneous Finite Slab One Energy Group Eigenvalue* for the cases l CG, q CG, l-l SGSO, l-q SGSO, l-l SGSBR, q-q SGSBR, l-l SGSMLDG, l-q SGSMLDG and q-q SGSMLDG. The q-q SGSBR method produced nonsensible solutions for mesh divisions above 10.
the test case *Homogeneous Infinite Square One Energy Group Eigenvalue* and the spatial flux solution oscillated massively with an almost periodic nature). The l-l SGSBR and l-l SGMLDG methods have a second order convergence but give a less accurate answer than the l-l SGSO and even the l CG method. The l-q SGMLDG method also has a second order convergence with an more accurate answer than l CG method but less accurate than l-l SGSO method. The q-q SGSBR and q-q SGMLDG methods have a third order convergence but are less accurate than q CG method. The SGSBR full solution for this case was found to have no discontinuity inherent to it. Also the q-q SGSBR method produced non sensible results for mesh division cases greater than 10 elements.

The result that in 1D the l-l SGSO full solution was piece wise constant across an element and that the l-q SGSO full solution was linear discontinuous was unexpected. The mathematical reason for this is unknown. The SGSBR and SGMLDG l-l methods did not produce this effect. Their full solution was linear discontinuous albeit less accurate in a global integral (the $\text{Keff}$) sense. To ascertain that these effects were not due to a computational implementation error they were verified independently by Pain (2010) for a different 1D test case.

As a comparison the 2D model of this 1D test case was produced. Here only the mesh resolution in the x axis need be considered as the solution is flat in the y axis (being effectively infinite due to the reflective boundary condition and homogeneous material properties). The CG alone method for both l and q basis sets gives identical results between the 1D and 2D models (as expected). Figures 4.9 and 4.10 show the Keff convergence of the 2D model for the SGSO method in comparison to the 1D model for the SGSO and CG methods. Initially on the coarse mesh resolution the l-l and l-q SGSO 2D models show a larger error than the l-l SGSO 1D model. As the mesh is refined the l-q SGSO 2D model shows a third order convergence but is vastly less accurate than the l-q SGSO 1D model. The l-l SGSO 2D model initially shows a third order convergence then when the resolution surpasses 64 elements shows a 2nd order convergence. For 4 elements or more the l-l SGSO 2D model has a significantly smaller error than the l-l SGSO 1D model. For the 2D model it was found that the q-q SGSO method produced a non sensible result. The full solution in the x axis for the 2D model using the l-l SGSO method gave a linear discontinuous variation. The full solution
Figure 4.9: The $K_{eff}$ versus number of elements for the test case *Homogeneous Finite Slab One Energy Group Eigenvalue* for the cases 1 CG, q CG, l-l SGSO 1D, l-q SGSO 1D, l-l SGSO 2D and l-q SGSO 2D.
Figure 4.10.: The relative Keff error versus number of elements for the test case Homogeneous Finite Slab One Energy Group Eigenvalue for the cases l CG, q CG, l-l SGSO 1D, l-q SGSO 1D, l-l SGSO 2D and l-q SGSO 2D.
Figure 4.11.: The $K_{eff}$ versus number of elements for the test case *Homogeneous Finite Slab One Energy Group Eigenvalue* for the cases 1 CG, q CG, l-l SGSO 1D, l-q SGSO 1D, l-l SGSMLDG 1D, l-q SGSMLDG 1D, l-l SGSMLDG 2D, l-q SGSMLDG 2D.

in the x axis for the 2D model using the l-q SGSO method appeared to give a linear discontinuous variation also.

Figures 4.11 and 4.12 show the $K_{eff}$ convergence of the 2D model for the SGSMLDG method in comparison to the 1D model for the SGSO, SGSMLDG and CG methods. The initial coarse mesh results show unexplainable variation between the 1D and 2D models for the SGSMLDG method. As the mesh resolution increases the convergence rates and errors between the 1D and 2D are more similar. However, the spatial full flux variation (due to the sub grid scale component) of the l-q SGSMLDG 2D solution in the y axis was found to be not flat as it should be. Minor fluctuations occur for an unknown reason. This was not observed in the l-l SGSMLDG 2D solution.

This test case has discovered several issues associated with the SGS meth-
Figure 4.12: The relative $K_{eff}$ error versus number of elements for the test case *Homogeneous Finite Slab One Energy Group Eigenvalue* for the cases l CG, q CG, l-l SGSMLDG 1D, l-q SGSMLDG 1D, l-l SGSMLDG 2D and l-q SGSMLDG 2D.
ods proposed and as computationally implemented. These are summarised as follows.

1. In 1D the l-l SGSO full solution is piece wise constant and the l-q SGSO full solution is linear discontinuous, an order lower than expected in each case.

2. In 1D there was very little difference between l-q SGSO and q-q SGSO.

3. In 1D the l-q SGSBR produced non sensible results.

4. The SGSBR method produced solutions that had no inherent discontinuity.

5. In 2D the q-q SGSO method produced non sensible results.

6. In 2D the l-q and q-q SGSM-LDG solutions were fluctuating in the y axis when they should have been flat across.

7. Models set up in 1D and 2D to represent the same case did not give identical results for any of the SGS methods.

The issues associated with the SGSBR and SGSM-LDG methods could be due to the rather ad-hoc nature of their derivation in the sub grid scale formulation presented. Issues associated with the q-q SGS results could be due to the bubble function producing two identical (or very similar) lines of the matrix equation as there is an identical weight function of both components being used. The first and the last issue associated with the SGSO method can not be explained.

This test case has also shown the benefit from the perspective of improved numerical accuracy of the SGSO method. The l-l SGSO method was shown to reduce the error by around 70% compared to the l CG method and the l-q SGSO method was shown to be more akin, with respect to error, to the q CG method.

4.3.3. Homogeneous Finite Square Two Energy Group Eigenvalue

This test case has a finite square domain with an outer zero flux boundary condition. There is one homogeneous material with two energy groups.
The material properties are taken from one of the materials in the LRA neutron kinetics benchmark Smith (1979) and are representative of a BWR fuel assembly. The material properties for this problem are given in Table 4.2. The size of the square was chosen such that the exact diffusion answer using these material properties would give a Keff of unity. Two geometric models are produced and compared against each other. The first represents the whole domain while the second models a quarter and uses a reflective boundary condition. These two geometric models are illustrated in Figure 4.13. Note that the first model has an zero boundary condition on all off the outer domain. Therefore there is no inconsistency with the inner element weak zero boundary condition that is applied in the various SGS methods. The quarter square model is used to test for inconsistency using an outer reflective condition. Both geometric models have their domains partitioned with structured quadrilateral elements. Mesh divisions are uniform and equal in each coordinate direction.

It was discovered that the q-q SGSO, q-l SGSO and l-q SGSBR produced non-sensible results. Also, the q-q SGSBR method produced non-sensible results on certain meshes. Figures 4.14 and 4.15 show the Keff convergence for the l CG , q CG , l-l SGSO and l-q SGSO methods with respect to the number of uniform divisions of the mesh in each coordinate direction. The l-l SGSO method for this test case is observed to converge from above. Recall that for the previous 1D test case this method converged from below for both 1D and 2D models. The l-l SGSO and l-q SGSO methods show a third order convergence with respect to mesh size and both have a more accurate Keff than the l CG but less accurate the q CG. The errors for the 5x5 mesh are shown in Table 4.3. The l-l SGSO method has an error an order of magnitude

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Table 4.2: Material properties of the test case Homogeneous Finite Square Two Energy Group Eigenvalue.
Figure 4.13.: The two geometric models used for the test case *Homogeneous Finite Square Two Energy Group Eigenvalue*. 

(a) 

(b) 

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Figure 4.14.: The Keff versus number of mesh divisions in each coordinate direction for the test case *Homogeneous Finite Square Two Energy Group Eigenvalue* for the cases l CG, q CG, l-l SGSO and l-q SGSO 1D.
Figure 4.15.: The relative Keff error versus number of mesh divisions in each coordinate direction for the test case Homogeneous Finite Square Two Energy Group Eigenvalue for the cases l CG, q CG, l-l SGSO and l-q SGSO 1D.
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<tr>
<td>l-l SGSO</td>
<td>$1.146158E - 4$</td>
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<tr>
<td>l-q SGSO</td>
<td>$5.165520E - 5$</td>
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Table 4.3.: Relative Error of the Keff for the SGSO method for the test case Homogeneous Finite Square Two Energy Group Eigenvalue compared to the CG method for the 5x5 mesh.

less than the 1 CG method being around 20 times smaller. The l-q SGSO method has an error around 40 times smaller than the 1 CG method. Recall that in principle the 1 CG, l-l SGSO and l-q SGSO methods should have similar computational work associated with them. The q CG method has the lowest error although this has a greater number of unknowns within the global matrix solver which for a 5x5 mesh is 36 unknowns for a 1 mesh and 121 for a q mesh. Considering this the errors for 121 unknowns into the global matrix solver are shown in table 4.4. From this perspective the l-l

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</tr>
<tr>
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Table 4.4.: Relative Error of the Keff for the SGSO method for the test case Homogeneous Finite Square Two Energy Group Eigenvalue compared to the CG method for 121 unknowns into the global matrix solver.

and l-q SGSO methods are superior to the q CG method with errors around half the size. The spatial flux plots for the l-l SGSO and l-q SGSO using a 5x5 mesh showing the full flux, the two components and the ratio of the sub grid scale component to the full solution are presented in figures 4.16 and 4.17 respectively for group 1. The group 2 flux in each case has a very similar spatial shape as that of group 1 and need not be shown. The l-l SGSO full solution has significant discontinuity whereas the l-q SGSO full solution in comparison has very little. The solution at the boundary can be
seen to be dominated by the sgs component in both cases.

Figures 4.18 and 4.19 show the Keff convergence for all the possible methods that produced sensible results for this test case. As in the previous test case the l-l SGSBR and l-l SGSMLDG methods have a second order convergence, convergence from above and have a less accurate answer than the l CG method. The l-q SGSMLDG method has second order convergence with an smaller error than the l CG method but is not as accurate as the SGSO methods. The q-q SGSMLDG method offers no improvement over the q CG method.

This test case has discovered a few more issues associated with the SGS methods proposed and as computationally implemented. These are summarised as follows.

1. The q-l SGSO method produced non sensible results.
2. The q-q SGSO method produced non sensible results.
3. The SGSBR method had no discontinuity within the full solution.
4. The l-q SGSBR method produced non sensible results.
5. The q-q SGSBR method produced non sensible results.

The issues associated with the SGSBR method, as mentioned for the previous test case, could be due to the ad-hoc nature of its derivation in the sub grid scale formulation presented. Due to the issues associated with the SGSBR method in this test case and the previous (including the accuracy and convergence) it will not be investigated in the following test cases. Similarly, due to the issues associated with the q-q SGS method in this test case and the previous (including the accuracy and convergence) it will not be investigated in the following test cases. The issue associated with the q-q SGSO method could be due to the use of the bubble function twice as a weight. The issue associated with the q-l SGSO method can not be explained however this is not a method of interest.

This test case has also shown the benefit from the perspective of improved numerical accuracy of the SGSO method. The l-l SGSO method was shown to reduce the error by one order of magnitude (being around 20 times less) compared to the l CG method for a 5x5 mesh. On a 10x10 mesh the error of the l-l SGSO method was around 85 times smaller than the l CG method.
Figure 4.16.: The spatial flux plots for the test case *Homogeneous Finite Square Two Energy Group Eigenvalue* for the case l-l SGSO for group 1. Shown from top to bottom is the full flux, cg component, sgs component and ratio of sgs component to full flux.
Figure 4.17.: The spatial flux plots for the test case *Homogeneous Finite Square Two Energy Group Eigenvalue* for the case l-q SGSO for group 1. Shown from top to bottom is the full flux, cg component, sgs component and ratio of sgs component to full flux.
Figure 4.18.: The $K_{eff}$ versus number of mesh divisions in each coordinate direction for the test case *Homogeneous Finite Square Two Energy Group Eigenvalue* for the cases l CG, q CG, l-l SGSO, l-q SG SO, l-l SGSM LDG, l-q SGSMLDG, q-q SGSMLDG, l-l SGSBR and q-q SGSBR.
Figure 4.19.: The relative $K_{eff}$ error versus number of mesh divisions in each coordinate direction for the test case *Homogeneous Finite Square Two Energy Group Eigenvalue* for the cases $l$ CG, $q$ CG, $l$-l SGSO, $l$-q SGSO, $l$-l SGSMLDG, $l$-q SGSMLDG, $q$-q SGSMLDG and $l$-l SGSBR.
This improvement with increased mesh resolution was shown to give the l-l SGSO method in this test case third order convergence. The l-q SGSO method was also shown to have third order convergence and for the same number of unknowns into the global solver to have a smaller error than the q cg method (3.6 times smaller for 121 unknowns on a 10x10 mesh).

This test case also showed that the use of a reflective boundary condition on the outer domain as implemented via not applying this to the SGS component produced no extra error for a 2D problem using structured quadrilateral elements.

4.3.4. BWR 2D Two Energy Group Eigenvalue

This test case is 2D quarter core representation of a Boiling Water Reactor (BWR). It consists of multiple materials with a two energy group structure. It is an international recognised benchmark for the static and transient comparison of numerical methods to solve the multigroup neutron diffusion equations with realistic geometries and materials Song and Kim (1992). Only the eigenvalue problem is considered here. The Analytic Nodal code PANTHER BE is used to provide a reference answer. PANTHER is an industry standard code used within the UK for whole core analysis. It has been extensively verified and validated for this purpose. This test case is one of the examples provided with the code. The actual benchmark specification is for a 2D and 3D geometry. Material properties are given for the 3D geometry in the literature. To apply the 2D model an extra absorption is needed within the materials to account for axial leakage. The extra absorption used here was taken from the PANTHER input file that is supplied with the code. The power densities for each PANTHER node (being a volume region representing a fuel assembly) are compared to the corresponding power density region averages of the CG and SGS methods. As there are 121 average regions with 78 of them fuelled relative error norms associated with the power density are used.

The $L_2$ error norm of power density $\|e_p\|_{L_2}$ is given by

$$\|e_p\|_{L_2} = \left( \int_{\Omega} (P_{\text{exact}} - P)^2 d\Omega \right)^{0.5},$$

where $P_{\text{exact}}$ and $P$ are the exact and approximate power density spatial...
distribution respectively. The dimensionless relative percentage $L_2$ error norm of power density $\eta_{L_2}$ is then given by

$$\eta_{L_2} = \frac{\|e_p\|_{L_2}}{\|P\|_{L_2}} \times 100,$$

(4.86)

where

$$\|P\|_{L_2} = \left( \int_{\Omega} P_{\text{exact}}^2 d\Omega \right)^{0.5}.$$

(4.87)

Similarly, the $L_1$ error norm of power density $\|e_p\|_{L_1}$ is given by

$$\|e_p\|_{L_1} = \int_{\Omega} |P_{\text{exact}} - P| d\Omega,$$

(4.88)

where $P_{\text{exact}}$ and $P$ are the exact and approximate power density spatial distribution respectively. The dimensionless relative percentage $L_1$ error norm of power density $\eta_{L_1}$ is then given by

$$\eta_{L_1} = \frac{\|e_p\|_{L_1}}{\|P\|_{L_1}} \times 100,$$

(4.89)

where

$$\|P\|_{L_1} = \int_{\Omega} |P_{\text{exact}}|^2 d\Omega.$$

(4.90)

Also, the $L_\infty$ error norm of power density $\|e_p\|_{L_\infty}$ is given by

$$\|e_p\|_{L_\infty} = \max (|P_{\text{exact}}(r) - P(r)|) \quad \forall r \in \Omega$$

(4.91)

and the dimensionless relative percentage $L_\infty$ error norm of power density $\eta_{L_\infty}$ is then given by

$$\eta_{L_\infty} = \max \left( \frac{|P_{\text{exact}}(r) - P(r)|}{|P_{\text{exact}}(r)|} \times 100 \right) \quad \forall r \in \Omega.$$

(4.92)

The quarter core consists of 78 fuel assemblies surrounded by a water reflector. The 78 fuel assemblies consist of 4 types and are labelled as material 1 to 4. The water reflector is material 5. The 5 material properties for the two energy groups are shown in table 4.5. The corresponding geometry, material mapping and boundary conditions for this test case are shown in
The PANTHER solution used a structured quadrilateral mesh with node sizes of 15cm by 15cm corresponding to the base unit size of the material geometry being a fuel assembly. The FEM CG and SGS methods used a structured quadrilateral mesh with the coarsest resolution corresponding to that of the PANTHER reference solution. The mesh resolution was then increased and results are presented in the context of the number of equal mesh divisions in the x and y coordinate direction within a fuel assembly (or a PANTHER node).

This test case was discovered to be problematic for the SGSO method in that a non sensible solution was obtained. Close inspection of the convergence of the eigenvalue and eigenvector during the power iteration algorithm showed that initially the solution was converging sensibly. The solution then however goes unstable and produces non sensible results. This is illustrated in figure 4.21 which shows the Keff and relative change in Keff for each power iteration for the l CG and l-l SGSO method using the same fine mesh. Initially the SGSO method converges similarly to the CG method with the line plots overlapping. Just after around 300 power iterations the SGSO solution jumps over about 10 power iterations and then oscillates erratically about an unrealistic value for the problem. After some testing with simpler cases it was discovered that the SGSO method was unstable if the absorption coefficient into the matrix assembly (which will be the removal cross

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Table 4.5.: Material properties of the test case BWR 2D Two Energy Group Eigenvalue.
Figure 4.20.: The geometry, material mapping and boundary conditions for the test case BWR 2D Two Energy Group Eigenvalue.
Figure 4.21.: The $K_{ef}$ (top) and relative change in $K_{ef}$ (bottom) for each power iteration for the 1 CG and 1-l SGSO method using the same fine mesh for the test case BWR 2D Two Energy Group Eigenvalue.
section for each group) is small and that if it was zero then the SGS matrices where singular. Through essentially guessing it was found that the SGSMin method produced a stable answer if the minimum absorption coefficient into the $D$ matrix associated with the SGS formulation was set as $0.05\, cm^{-1}$ for this test case.

Figure 4.22 shows the convergence of the three defined relative percentage error norms for the l CG, q CG, l-l SGSMin, l-q SSGMin, l-l SGSMLDG and l-q SGSMLDG methods. The three different error norms all show the same relative behaviour between the different methods. All the SGS methods show improvement in the solution relative to the l CG method. The l-l SGSMin and l-q SGSMLDG methods have a convergence similar to the q CG method for the lower mesh divisions. With increased mesh divisions the l-l SGSMin method does not retain this rate and oscillates in convergence mildly. The full solution and sgs component for the thermal flux (group 2) is shown in figure 4.23 for the l-l SGSMin method with 3 mesh divisions. Prominent discontinuity in the flux is seen at the material - material interfaces with the sgs component almost tracing out the material boundaries.

The l-q SGSMLDG method shows a similar convergence behaviour to l-l SGSMin but with initially a higher error followed then by a lower error. The l-q SGSMLDG method gives the lowest error solution for 3 mesh divisions with the $L_\infty$ norm error being around $0.4\%$. In comparison to achieve this accuracy 4 mesh divisions were needed for the q CG method and with 10 mesh divisions the l CG method had a $L_\infty$ norm error around $0.9\%$. Even though the l-q SGSMLDG method appears as accurate as q CG, on inspection of the spatial flux solution oscillations exist within the sgs component that look almost structured or intended. They are however unrealistic. Whether these appear due to the formulation or the computational implementation is unknown. For this test case the l-q SGSMin method has a worse solution than the l-l SGSMin method although is still an improvement over the l CG method. This counter intuitive result can not be explained.

This problem is sufficiently large to compare the different methods with respect to computational time and memory. To compare the time profiles of the different methods profiling flags were included at code compile and the program $GPROF$ was used in the Linux terminal. Each case was run on the same workstation five times and the average time taken is used for the comparison. To compare the memory usage the Linux terminal program
Figure 4.22: The relative percentage $L_2$ norm error (top), the relative percentage $L_1$ norm error (middle) and the relative percentage $L_\infty$ norm error (bottom) of the power density for the test case BWR 2D Two Energy Group Eigenvalue for the l CG, q CG, l-l SGSMin, l-q SSGMin, l-l SGSMLDG and l-q SGSMLDG methods.
Figure 4.23.: The full solution and sgs component for the test case BWR 2D Two Energy Group Eigenvalue using the l-l SGSMin method with 3 mesh divisions.
TOP was used to obtain the virtual and resident memory. Absolute timings and memory are not relevant, only the relative comparison between the methods. Therefore the timings and memories are normalised such that the l CG method takes 1 unit time with 1 unit memory. Note that no relevant difference with respect to timings and memory was found between the different SGS methods.

Irrespective of the solution error the methods are initially compared for the 10 mesh divisions case. Table 4.6 shows the normalised computational timings and table 4.7 shows the normalised memory usage. These tables show that the l-l SGS methods increase the computational requirement (time and memory) by about 50% relative to the l CG method for the same mesh for this test case. The l-q SGS methods increase this by around 150% compared to the l CG method but compared to the q CG method use about the same memory and are around 5.5 times faster. The l-l SGS and l-q SGS methods were found to have required the same number of solver (inner and power) iterations as the l CG method.

A more fairer comparison would take account of the solution error. The previous results showed that the l CG solution with 10 divisions had a similar error to that of the q CG and l-l SGSMin methods with 3 mesh divisions.
The average timings and memory usage for these three cases are shown in tables 4.8 and 4.9 respectively. Again each was normalised such that the l CG method was unity. These tables show that for around the same error

<table>
<thead>
<tr>
<th>Method</th>
<th>Normalised Average CPU Timings</th>
</tr>
</thead>
<tbody>
<tr>
<td>l CG</td>
<td>1.0</td>
</tr>
<tr>
<td>q CG</td>
<td>0.052</td>
</tr>
<tr>
<td>l-l SGS</td>
<td>0.098</td>
</tr>
<tr>
<td>PANTHER (1 run)</td>
<td>0.0216</td>
</tr>
</tbody>
</table>

Table 4.8.: Normalised average CPU timings for the test case BWR 2D Two Energy Group Eigenvalue for l CG with 10 mesh divisions, q CG with 3 mesh divisions and l-l SGS with 3 mesh divisions. Also shown is the normalised PANTHER time taken from one run.

<table>
<thead>
<tr>
<th>Method</th>
<th>Normalised Resident Memory</th>
<th>Normalised Virtual Memory</th>
</tr>
</thead>
<tbody>
<tr>
<td>l CG</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>q CG</td>
<td>0.577</td>
<td>0.914</td>
</tr>
<tr>
<td>l-l SGS</td>
<td>0.635</td>
<td>0.92</td>
</tr>
</tbody>
</table>

Table 4.9.: Normalised memory usage for the test case BWR 2D Two Energy Group Eigenvalue for l CG with 10 mesh divisions, q CG with 3 mesh divisions and l-l SGS with 3 mesh divisions.

the l-l SGS method is about 10 times faster than l CG and q CG is about 20 times faster than l CG. Also shown is the time taken for the reference PANTHER solution. This number was taken from the standard PANTHER output file for one run and so was not calculated in exactly the same way as the other methods. The PANTHER simulation was run on a different workstation to the other methods. This workstation was consistently shown to be about twice as slow and this is taken into account in calculating the relative PANTHER simulation time. This number should therefore be taken as a rough estimate of the time taken. Also the PANTHER solution is the reference so has no error like the other methods and is hence more accurate. The PANTHER solution was calculated about 50 times faster than the fine mesh (but not fully spatially converged) l CG solution presented. The q CG and l-l SGS methods offer about a 40% saving in resident memory compared to the l CG method for around the same error for this case.
4.4. Conclusions

This chapter presented a recently developed inner element sub grid scale finite element method applied in the context of multigroup neutron diffusion. The method decomposes the full solution into a continuous global and inner element sub grid scale components. The continuous global component has an identical formulation to the standard Continuous Galerkin method. The inner element sub grid scale component enriches the solution locally and is naturally discontinuous across element-element boundaries. The extra discretised sub matrices associated with sub grid scale formulation are element wise block diagonal. This allows for an efficient element wise static condensation algorithm to be employed. The resulting global linear system to be solved for requires the same computational work as that inherent to the standard Continuous Galerkin method.

The formulation of the method was shown followed by a description of a simplification of the outer domain boundary condition. A couple of different methods of treating the diffusion term of the sub grid scale component were introduced in an manner as to have some similarities to those used in Discontinuous Galerkin methods. These were introduced as stability issues were encountered with the original derived formulation.

To analyse the capabilities of the method it was applied to a small range of eigenvalue test cases in one or two energy groups. Only problems using structured meshes were considered.

The initial test case was used to purely check that the sub grid scale parts of the method were capable of doing nothing, which they did.

The second test case analysed the method in 1D slab geometry with one energy group. Errors and orders of convergence were investigated. What was termed the original method (SGSO) was found capable of reducing the error by around 70% in comparison to the standard Continuous Galerkin (CG) method using linear (l) Lagrange basis functions for both components. To achieve a Keff relative error of around 1pcm the l-l SGSO method was found to require half the number of spatial elements. The l CG and l-l SGSO methods were found to have second order Keff convergence for this test case. The q CG and l-q SGSO methods were found to have third order Keff convergence with respect to number of elements. From the number of elements perspective the q CG method was most accurate whereas from the
number of unknowns into the continuous component linear algebra solver the l-q SGSO method was most accurate. The alternative methods (SGSBR and SGSMLDG) of treating the diffusion term did not have much success for this test case. Several issues were discovered associated with the various SGS methods for this test case. Only speculative reasons could be given for these issues.

The third test case analysed the method in 2D XY geometry with two energy groups. Again more issues associated with the SGS methods as computationally implemented were found. This led to the conclusion that from these few results given that the SGSBR method was a poor method that was shown to produce a worse solution than CG. Also, the conclusion was reached that using quadratic basis functions on both components of the SGS methods may have a formulation issue. However, the l-l SGSO method was shown to have third order convergence and an error over an order of magnitude less than the l CG method for this test case. Also, the l-q SGSO method was shown to have third order convergence and to be more than three times more accurate than q CG with respect to the number of unknowns into the continuous component solver. This test case also showed that no error was incurred through the application of the simplified outer domain boundary condition.

The fourth and final test case was a 2D two group international neutron kinetics benchmark representative of a BWR core. The industrial Analytic Nodal code PANTHER was used to generate a reference solution. Error norms of the spatial power density were used to analyse the SGSMin and SGSMLDG methods. The SGSO method was shown to be unstable for this problem and stated to produce singular matrices if the absorption coefficient (being the removal cross section) is zero. The l-l SGSMIn and l-q SGSMLDG methods were shown to be as accurate as the q CG method at low mesh divisions. The l-q SGSMIn and l-l SGSMLDG methods were not as accurate but still showed an improvement over the l CG method. Computational time and memory usage for the different methods was then discussed. Both l-l SGS methods were shown to require about 50% more time and memory in comparison to l CG for the same mesh resolution. The l-q SGS method was shown to require about 150% more for the same case. For the same solution error the l-l SGS was then shown to require about 10% of the time taken by the l CG method. In comparison the q CG required about 5% of
the time taken by the l CG.

In conclusion the original SGSO method proposed generally showed beneficial characteristics in comparison to the standard CG method. However, the method was shown to have stability issues via direct application. Alternative methods to avoid this were analysed but tended to have poor convergence traits in comparison to the CG and SGSO method. A more rigorous mathematical derivation of a stable alternative that maintained (or improved on) the original method presented accuracy would be a suggestion for future research. Also an investigation in to the use of different shape function orders and families could be considered. This would not only benefit the application of the method in a neutron diffusion context but in any general context where the method is applied to an advection-diffusion equation. Further investigation of the method is also needed when applied to unstructured meshes and time dependent problems. If a stable method is obtained then the method could be easily extended to solve the second order even parity neutron transport equation or the simplified Pn equations. Also the method would be applicable as part of a diffusion acceleration scheme to a DG or SGS first order transport method.
Chapter 5

Very High Temperature Reactor Radiation Transport Modelling

Synopsis

A range of radiation transport models of the block type Very High Temperature Reactor are developed and used to analyse the design. The primary aim is develop a whole core 3D FETCH model that is suitable for coupled steady state and transient simulations. Therefore solution error must be quantified with regard to spatial, energy and angle approximations. Due to the vast degree of heterogeneity inherent within the design the deterministic FEM based FETCH model requires homogenisation in space and energy. The reactor physics code WIMS9 is used to generate homogenised material properties for the FETCH models. A Monte Carlo based MONK9 model is also developed which represents the spatial and energy heterogeneity as best as possible. The range of increasing complexity models developed are cross compared between WIMS9-FETCH and MONK9, with the MONK9 model taken as a more accurate reference. Initially a WIMS9-FETCH RZ model of the HTR-10 pebble bed IAEA reactor benchmark is analysed to provide evidence to support model validation.
5.1. Introduction

In this chapter a range of increasing complexity radiation transport models of a generic VHTR are developed. The primary purpose is to develop a whole core FEM based FETCH model that is suitable for coupled radiation transport thermal fluid dynamic analysis. An RZ and two XYZ FETCH models are developed for comparison. Different meshes resulting in different material representations are also developed for the XYZ model. Convergence in the spatial, energy and angle discretisation is analysed to quantify solution error. A two step homogenisation process is used whereby the heterogeneity is represented as best as possible in the reactor physics code WIMS9 ANSWERS-WIMS to produce homogeneous material properties for
the whole core FETCH models. A substantially more spatially detailed range of models are also developed using the Monte Carlo based MONK9 ANSWERS-MONK code that uses a continuous energy representation for cross sections. Comparisons are made between the WIMS9-FETCH models and the MONK9 models where the MONK9 model is considered the more accurate and taken as a reference. These comparisons involve only the criticality factor $K_{ef}$. Different models used within WIMS9 are investigated to show that for the design considered the simpler option was suitable. This analysis considered a uranium fuelled core with no burn up. Different fissile materials or inclusion of burnup may require the more detailed model within WIMS9. Due to both the WIMS9-FETCH and MONK9 models producing results that had too high an excess reactivity, variations to the design are considered via reducing the enrichment.

Initially the WIMS9-FETCH combination model is partially validated via application to the HTR-10 pebble bed IAEA benchmark for initial criticality IAEA-TECDOC-1382 (2003). Here an RZ model is developed and spatial and energy convergence investigated. To obtain a more accurate result streaming correction factors were needed due to the small size of the core. These are applied as directionally dependent diffusion coefficient corrections in the parallel and perpendicular directions to the streaming channels. The modelling of the HTR-10 is chosen for two reasons. First the review report Terry et al. (2004) concludes that for the validation of the codes used in the development of the U.S.A. VHTR design (usually referred to as the Next Generation Nuclear Reactor, NGNP) the most suitable existing experimental data comes from the HTR-10 and the Japanese HTTR. This was mainly because they both used low enriched Uranium and are operational. Both were included as benchmarks in the IAEA report IAEA-TECDOC-1382 (2003). With only time to model one of them the HTR-10 is chosen as the benchmark results were more accurate than the HTTR. Errors arose in the HTTR benchmark due to burnable poisons and annular core configurations. Also there appeared to be insufficient data within the report IAEA-TECDOC-1382 (2003) with regard to benchmark definition changes for the HTTR.

This chapter is organised as follows. In the first section the WIMS9-FETCH two step model is applied to the HTR-10 benchmark to provide evidence to support validation. Following this the general VHTR design
considered is described. The range of MONK9 models that were developed are then described and results presented. Then the WIMS9 models used to produce homogenised cross sections are presented with results. The whole core FETCH models are then described. Results from the various whole core FETCH models are analysed and compared to the MONK9 results. Control rod worth, $K_{\text{eff}}$ and power densities are presented. Finally conclusions are stated as to the suitability of the WIMS9-FETCH models to capture the physics of interest.

Unless stated the convergence tolerances used within EVENT and BEANS for the inner and outer iterations should be assumed as $1.0E^{-08}$.

5.2. HTR-10 WIMS9-FETCH Model

In a previous chapter 3 a case was made to provide evidence of verification of the neutronic codes EVENT and BEANS that are part of FETCH. Sufficient test examples were included within an automated framework to state that these two codes are functioning as intended. All the test cases previously mentioned where predominantly characteristic of Light Water Reactors and none were VHTR relevant solution verification or validation tests. Therefore to provide some partial validation evidence of EVENT and BEANS for VHTR modelling the HTR-10 IAEA initial criticality benchmark IAEA-TECDOC-1382 (2003) was used. The validation test was to deduce the initial critical height of the pebble bed. The test case also involved the calculation of control rod worth and variation of $K_{\text{eff}}$ with changes in core temperature. These are however considered verification tests as comparison is made to the other model results only. Experimental results were presented for individual control rod worth but not obvious for all control rod worth together. To generate the homogenised material properties WIMS9 was used and is therefore involved in the validation process. WIMS9 itself has been used and tested on HTGR problems including international benchmarks and was used by one of the participants of this HTR-10 benchmark. Taking account of streaming in the empty control channels that surround the core was found to be important to achieve improved accuracy. This was captured through the use of anisotropic diffusion coefficients in BEANS generated using correction factors. Justification for the use of the Behrens (Appendix A) method to capture this channel streaming effect is shown via
comparison with a MONK model for a simplified reactor geometry of the HTR-10. This is given in Appendix D.

5.2.1. HTR-10 Benchmark Definition

The RZ model geometry and materials used were that specified in the benchmark definition. The model geometry is shown in figure 5.1 where the region numbers signify the material mapping of different graphite reflector and carbon brick insulator regions. The radius of the pebble bed is 90cm and the initial core height to achieve criticality was around 123cm. The benchmark document states that the initial model specification and actual experiment had slight deviations and some results were repeated with the more relevant conditions. This included the correct temperature of 15°C, the presence of air instead of helium and an increase in moderator pebble graphite density to 1.84 g/cc. Only the more relevant conditions that resembled the actual experiment are considered here in. The material number densities from the benchmark specification for the various reflector regions had been determined by volume smearing the various regions. This means that axial channel regions adjacent to the core have been initially averaged with surrounding graphite and this should be considered in the analysis. These streaming channels can be seen in figure 5.2 which shows an actual photo of the reactor core looking down into the cone region.

The initial core consisted of a mixture of fuel pebbles and dummy (all graphite) pebbles in a ratio of 57:43 respectively. The pebbles have a diameter of 6.0cm with the inner fuelled region diameter being 5.0cm. The heavy metal loading per fuelled pebble was 5 grams with a U235 enrichment of 17%. The cone region below the active core is filled solely with dummy graphite pebbles. The control rod is presumed inserted to a depth of 114.7cm in the side reflector from the top which places the tip above the active core height.

5.2.2. HTR-10 WIMS9 Models

To produce homogenised fuel and cone region cross sections a simplified geometry within WIMS9 is used to provide a flux solution that is used to flux weight smear as needed. The WIMS9 modules used for this process are HEAD - PRES - PROC - RES - PIP - SMEAR. The HEAD module
Figure 5.1.: HTR-10 IAEA benchmark geometry IAEA-TECDOC-1382 (2003).
Figure 5.2.: HTR-10 photo of core region surrounded by reflector blocks with visible streaming channels Lohnert (2007).
interpolates in temperature the necessary cross sections from the 172 group library. The PRES - PROC - RES sequence then corrects these 172 group cross sections for spatial and energy self shielding using a sub group approach. PROC uses a collision probability method that accounts for the double heterogeneity in the fuelled region of the pebble. PIP then uses the resonance shielded cross sections to calculate a 172 group flux solution that is used for the flux weighted smear of the active core region and the cone region below.

The geometry used in HEAD for the core region model is of a single TRISO particle kernel surrounded by shells of the corresponding volume per TRISO particle of fuel pebble graphite moderator, air gap and then dummy graphite pebble. The geometry used within PROC for the core region is of a fuelled pebble surrounded by the corresponding volume per fuelled pebble of air gap and dummy graphite pebble. The spherical radius calculated for each of these two models compares very closely with that of participants in the benchmark report IAEA-TECDOC-1382 (2003), as does the calculated number density for the core materials.

To produce smeared control rod cross sections an identical model to that described by the German institute (Research Centre Julich) within IAEA-TECDOC-1382 (2003) is used. This entailed an axially homogenised model of a control rod surrounded by a reflector region and then a ring of the smeared core region to act as a driver to generate an appropriate flux needed for the flux weighted smear. The WIMS9 module PIJ was used to generate the collision probabilities which were then solved by PIP. The maximum of 200 region divides was used across the PIJ model.

The HEAD module is used to interpolate as needed the various graphite reflector region materials. The smeared core material, smeared cone material, smeared control rod material, reflector material and the air material used in the core WIMS9 model are then output from WIMS9. A PYTHON script, WIMS2BEANS.py, is used to process the WIMS9 output file to produce the material input files for EVENT and BEANS. The multigroup diffusion coefficient that is used within BEANS is calculated from the multigroup transport cross section generated by WIMS9. The PYTHON script was verified by comparison of the input and output files. This PYTHON script applies streaming corrections to the pebble bed and reflector regions that contain axial channels. The pebble bed (core and cone) regions have the isotropic
Liebroth correction Liebroth and Stojadinovic (1980) applied and the reflector channel regions (being control rod, boron ball and inlet helium) have the anisotropic Behrens correction applied (described in Appendix A). These correction correlations are only applicable to diffusion coefficients hence the EVENT model cannot use them whereas the BEANS model can.

Note that the cross sections output from WIMS9 are in 172 groups form. No flux condense was performed using WIMS9 for this case. Also all cross sections were generated at a temperature of 15 C for the initial criticality test. The core (active region, cone and upper plenum) cross sections were then generated also at 20, 120 and 250 C retaining the air atmosphere.

5.2.3. HTR-10 RZ FETCH Model

The RZ geometric FETCH model (produced by GEM) is identical to that of the benchmark specification and shown in figure 5.3. This figure shows the lowest resolved mesh needed to define the material regions including the cone. Due to the large number of materials the colour scheme is not very clear. The cone region is represented as required and the regions are meshed with quadrilaterals. Most of the mesh is Cartesian grid aligned apart from the regions above and below the slanted cone interface. Vacuum boundary conditions are applied to the outer surfaces. Simulations are performed for 172 groups in BEANS and EVENT comparing the use of P1 scatter data in EVENT to transport cross sections in BEANS when no streaming corrections are applied. The 172 group solution in BEANS for a mesh size of around 5cm (5318 volume elements) is used to flux condense all the material regions to 11 groups with the upper group boundaries being 17, 31, 45, 61, 92, 116, 126, 140, 148, 157 and 172. The pebble bed height for the 172 group calculation here is at 123.06cm which is the experimentally determined critical height. Note that the diffusion coefficient is flux condensed retaining the anisotropic streaming corrections. The 11 group material data is then used to analyse the mesh convergence of the BEANS model and to determine the critical height. The mesh that produces an acceptable converged accuracy with 11 groups is then used for the 172 group RZ analysis that follows. Note that WIMS9 could have been used to condense the cross sections but the FETCH 172 group diffusion models were found to take a few minutes to complete, only a few eigenvalue calculations were needed and condensing in
Figure 5.3: HTR-10 RZ FETCH geometry model shown with lowest resolution mesh needed to define the regions. The colours represent different materials that are illustrated by the region numbering in figure 5.1.
WIMS9 would incur more error. The Keff for varying core temperature is determined using 172 groups with a full core height of 180.12cm. The control rod worth is determined using 172 groups using a close to initial core height of 126.0cm at a temperature of 15°C.

5.2.4. HTR-10 WIMS9-FETCH Results

Initially the $K_\infty$ from the infinite unit cell WIMS9 calculation for the core region is compared to the other presented values in the literature. Results are presented in table 5.1, where the results from France and Germany are from IAEA-TECDOC-1382 (2003) and the results from the Netherlands from Boer (2009). The Netherlands result was calculated using SCALE at 27°C and the German result calculated using VSOP at 20°C with the unchanged original benchmark specification. The French result for the heterogeneous model used the updated more relevant data and is considered to have the used the most accurate method (Monte Carlo code TRIPOLI4) so is taken as the reference which the others are compared to. The French result for the homogeneous unit cell also used the updated data and the deterministic code APOLLO to smear the geometry. The larger error associated with the German result is considered due to this result using the original benchmark data, use of the updated data generally caused the criticality factor to increase. The WIMS9, SCALE and heterogeneous TRIPOLI results generally agree within 170pcm of each other with both the WIMS9 and SCALE results being within one standard deviation of the TRIPOLI results (the standard deviation being 0.00125). This is an important verification result for the use of WIMS9 to model the basic unit cell of the core.

| Method               | $K_\infty$ | $|\Delta K_\infty/K_\infty|_{ref}$ |
|----------------------|------------|----------------------------------|
| WIMS9 (author UK)    | 1.759515   | 1.1552E-03                       |
| SCALE (Netherlands)  | 1.7625     | 5.3930E-04                       |
| VSOP (Germany)       | 1.7475     | 7.9759E-03                       |
| TRIPOLI Hom (France) | 1.76431    | 1.5668E-03                       |
| TRIPOLI Het (France) | 1.76155    | 0.0                              |

Table 5.1.: The $K_\infty$ and relative error for the HTR-10 core unit cell models where the heterogeneous TRIPOLI4 results is taken as the reference.
The results comparing EVENT to BEANS for a mesh resolution of 5318 volume linear elements that are roughly of size 5cm where no streaming corrections are considered are shown in table 5.2. For these simulations the bed height was set to the experimentally determined critical height of 123.06cm and 172 groups were used. The relative difference between Keff’s

<table>
<thead>
<tr>
<th>Method</th>
<th>Keff</th>
</tr>
</thead>
<tbody>
<tr>
<td>EVENT P1P0</td>
<td>1.0518207</td>
</tr>
<tr>
<td>BEANS P1P0</td>
<td>1.0518190</td>
</tr>
<tr>
<td>EVENT P1P1</td>
<td>1.0292451</td>
</tr>
<tr>
<td>BEANS P1Tr</td>
<td>1.0289992</td>
</tr>
<tr>
<td>EVENT SP3P1</td>
<td>1.0310211</td>
</tr>
<tr>
<td>EVENT SP5P1</td>
<td>1.0310197</td>
</tr>
<tr>
<td>EVENT P3P1</td>
<td>1.0353709</td>
</tr>
</tbody>
</table>

Table 5.2: The Keff for the HTR-10 RZ EVENT and BEANS models for different angular approximations (flux expansion then scatter kernel expansion where Tr refers to the use of transport cross sections). No streaming corrections are considered, the pebble bed height was 123.06cm and 172 groups was used.

(\Delta) are now discussed where the relative difference is calculated by

\[
\Delta = \frac{K_{eff_{ref}} - K_{eff}}{K_{eff_{ref}}},
\]

where \(K_{eff_{ref}}\) is the reference Keff chosen as the theoretically more accurate answer.

Agreement between EVENT and BEANS for the P1PO (P1 flux and P0 scatter kernel) is within a relative difference of \(1.6E-06\) as expected.

The relative Keff difference between the EVENT P1P0 and P1P1 (isotropic scatter compared to linear anisotropic scatter) is \(2.2E-02\). The P1P1 Keff is lower than the P1P0 result as the linear anisotropic scatter increases the forward direction scatter of neutrons thereby increasing the leakage from the core.

The relative Keff difference between the EVENT P1P1 and the BEANS P1Tr is \(2.34E-04\) showing that the approximation in using transport cross sections is acceptable.
The relative Keff difference between the EVENT P1P1 and EVENT SP3P1 is $1.72E - 03$. The relative Keff difference between the EVENT P1P1 and EVENT P3P1 is $5.92E - 03$. Little difference exists between the EVENT SP3P1 and EVENT SP5P1 Keff. Transport effects associated with the core reflector interaction thus cause the estimated Keff to increase. Higher order Pn flux solutions were not possible due to the gas cavity region above the core causing the EVENT solver difficulty with convergence.

The BEANS P1Tr 172 group flux solution for the roughly 5cm linear element mesh with a pebble bed height of 123.06cm and using the streaming corrections was used to flux weight condense the material properties to 11 groups. The 11 group upper group boundaries were 17, 31, 45, 61, 92, 116, 126, 140, 148, 157 and 172. The difference in Keff between the 172 group and 11 group BEANS P1Tr was about 40pcm. The 11 group RZ BEANS mesh was then varied to investigate spatial solution convergence. Results are shown in table 5.3 for the use of linear and quadratic basis functions. The relative Keff error uses the finest (21272 volume elements) quadratic solution as the reference. Mesh A refers to the minimum mesh constructed to resolve the material geometry and corresponds to that shown in figure 5.3. Mesh B refers to a selectively slightly refined mesh shown in figure 5.4.

The superior convergence rate of the quadratic basis functions compared

<table>
<thead>
<tr>
<th>Mesh</th>
<th>Volume Elements</th>
<th>Basis Order</th>
<th>Keff</th>
<th>Rel. Keff Error</th>
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<tr>
<td>A</td>
<td>212</td>
<td>linear</td>
<td>0.91511</td>
<td>7.9116e-01</td>
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<tr>
<td>B 10cm</td>
<td>343</td>
<td>linear</td>
<td>0.98455</td>
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<td>5318</td>
<td>linear</td>
<td>0.99132</td>
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<td>linear</td>
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<td>1.2455e-04</td>
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</table>

<table>
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<tr>
<th>Mesh</th>
<th>Volume Elements</th>
<th>Basis Order</th>
<th>Keff</th>
<th>Rel. Keff Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>212</td>
<td>quadratic</td>
<td>0.99296</td>
<td>7.799e-04</td>
</tr>
<tr>
<td>B 10cm</td>
<td>343</td>
<td>quadratic</td>
<td>0.99296</td>
<td>7.720e-04</td>
</tr>
<tr>
<td>B 5cm</td>
<td>1382</td>
<td>quadratic</td>
<td>0.99311</td>
<td>6.248e-04</td>
</tr>
<tr>
<td>B 2.5cm</td>
<td>5318</td>
<td>quadratic</td>
<td>0.99350</td>
<td>2.342e-04</td>
</tr>
<tr>
<td>B 1.25cm</td>
<td>21272</td>
<td>quadratic</td>
<td>0.99373</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Table 5.3.: The Keff for the HTR-10 RZ BEANS 11 group model for different spatial approximations. Streaming corrections are applied and the pebble bed height is set to 123.06cm. The 11 group cross sections were flux condensed from a 172 group RZ BEANS model.
Figure 5.4: HTR-10 RZ FETCH model shown with a selectively slightly refined mesh giving 343 volume elements. The colours represent different materials that are illustrated by the region numbering in figure 5.1.
to the linear is evident. A reasonable $K_{\text{eff}}$ is shown for both Mesh A and Mesh B using quadratic basis functions. Mesh B is used for the benchmark analysis in 172 groups. Mesh B is chosen over Mesh A as the increased number of divides axially will mean a more resolved control rod position using the control rod algorithm. The control rod algorithm (described in Appendix B) is used to place the rod bank in determining the control rod worth.

The 172 group 5cm mesh BEANS model was compared with and without applying the streaming corrections. The $K_{\text{eff}}$ with without streaming corrections was 1.02900 and with streaming corrections 0.99220. This corresponds to a change in $K_{\text{eff}}$ of 0.0368 which is quite substantial and to a percentage change of about 3.58\% when applying the correction. The only comparison available for this was from the Monte Carlo results from the French participants of the benchmark that give a value of 2.38\% change (1.48\% for the reflector channels and 0.9\% for the pebble bed).

To determine the initial critical height the 11 and 172 group RZ BEANS P1Tr models with streaming corrections using Mesh B were varied. The results are shown in figure 5.5. From these results the 11 group solution estimates an initial critical height of 125.9cm and the 172 group a height of 125.8cm. The BEANS result for initial critical height using 172 groups is compared to the benchmark document results IAEA-TECDOC-1382 (2003) in table 5.4. The BEANS result is the only one to overestimate the critical

<table>
<thead>
<tr>
<th>Participant</th>
<th>Estimate Critical Height (cm)</th>
<th>Relative Error (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>BEANS RZ</td>
<td>125.8</td>
<td>2.227</td>
</tr>
<tr>
<td>China D/T</td>
<td>122.558</td>
<td>0.408</td>
</tr>
<tr>
<td>China MC</td>
<td>122.874</td>
<td>0.151</td>
</tr>
<tr>
<td>France</td>
<td>117.37</td>
<td>4.624</td>
</tr>
<tr>
<td>Germany 2D</td>
<td>121.0</td>
<td>1.674</td>
</tr>
<tr>
<td>Germany 3D</td>
<td>123.3</td>
<td>0.195</td>
</tr>
<tr>
<td>Netherlands</td>
<td>122.1</td>
<td>0.780</td>
</tr>
<tr>
<td>S. Africa</td>
<td>122.537</td>
<td>0.425</td>
</tr>
<tr>
<td>Experiment</td>
<td>123.06</td>
<td>0.0</td>
</tr>
</tbody>
</table>

Table 5.4: A comparison of the estimates of the initial critical height of the HTR-10. The relative error is to that of the experiment. D/T refers to a combined diffusion transport method and MC to a Monte Carlo method.
Figure 5.5.: Variation of $K_{eff}$ with pebble bed height for the HTR-10 initial criticality estimate using the 11 and 172 group RZ BEANS models.
height and is not as close as other similar code results such as that used by the Netherlands participants. The error associated with the BEANS result could be due to:

- Discrepancies in the benchmark definition such as position of control rods.
- Homogenisation error of the pebble bed double heterogeneity and the control rods.
- Transport effects of the RZ model not resolved.
- Capturing streaming of neutrons in the pebble bed, reflector channels and the top cavity insufficiently.

The Keff for varying the core temperature at 20, 120 and 250 C using the WIMS9-BEANS model is compared to other available results in figure 5.6. Note that all the other results were obtained using different modules of the VSOP code. The WIMS9-BEANS results show a similar gradient to the German 2D and 3D results, albeit with each of these three being shifted axially to each other. The S. African and Chinese results show similar gradients to each other but with slightly lower gradient values than the WIMS9-BEANS and German results. The cause of the differences of this weak graph to graph verification could include that discussed previously, as well as due to:

- Discrepancies in the benchmark definition associated with which regions are increased in temperature, being the pebble bed, cone, cavity and reflector.
- The retaining of air rather than helium in the WIMS9-BEANS model.

The control rod worth percentage (CRW) is defined to be

\[
CRW = \left( \frac{1}{K_{eff_{rodin}}} - \frac{1}{K_{eff_{rodout}}} \right) \times 100. \quad (5.2)
\]

The CRW of all rods for the almost initial critical height of 126.0cm for the WIMS9-BEANS model is compared to other available results in table 5.5. The CRW is calculated from a rod in z axis height of -394.2cm to a rod out axis height of -230.318cm with respect to figure 5.1. Over a 60% difference is
Figure 5.6.: Variation of Keff with core temperature for the HTR-10 using the 172 group RZ BEANS model with a pebble bed height of 180.12cm.
<table>
<thead>
<tr>
<th>Participant</th>
<th>Control Rod Worth (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>WIMS9-BEANS</td>
<td>31.49</td>
</tr>
<tr>
<td>China D/T</td>
<td>17.23</td>
</tr>
<tr>
<td>China MC</td>
<td>18.28</td>
</tr>
<tr>
<td>France</td>
<td>13.80</td>
</tr>
<tr>
<td>Germany</td>
<td>19.31</td>
</tr>
</tbody>
</table>

Table 5.5.: A comparison of the estimates of the control rod worth of all rods for the almost initial critical height (126.0cm) of the HTR-10. D/T refers to a combined diffusion transport method and MC to a Monte Carlo method.

seen between the WIMS9-BEANS CRW and the Chinese CRW’s. Around a 25% difference is seen between the French and Chinese CRW’s. The causes of the large difference between WIMS9-BEANS and the Chinese results will be due to previously discussed reasons. The main reason is considered due to the geometric model and the method used to produce homogenised control rod region cross sections. An improved homogenisation method such as Super Homogenisation is expected to be capable of reducing this error and will be an option available in future WIMS versions.

5.2.5. HTR-10 Summary

A RZ FETCH model using homogenised cross sections generated by WIMS9 was used to perform part of the HTR-10 IAEA benchmark. The $K_\infty$ from the WIMS9 calculations showed close agreement to other available results being within one standard deviation of a Monte Carlo method solution. For a reasonable spatial resolution EVENT and BEANS were compared. Good agreement was achieved where expected. The capturing of anisotropic scatter was shown to be important and that the use of transport cross sections was shown accurate enough. A P3 EVENT calculation showed that the RZ geometry problem defined had some transport effects with some minor importance, but were less important than capturing anisotropic scatter and streaming effects. A 172 group BEANS solution was used to condense the cross sections to 11 groups which had a relative $K_{eff}$ difference less than 40pcm. The 11 group problem was used to investigate mesh convergence where quadratic basis functions were found to be very favourable with a
very coarse number of volume elements. A selectively chosen coarse mesh using quadratic basis functions was then used for the 172 group problem to determine the initial critical height, the Keff changes with temperature and the control rod worth. The WIMS9-BEANS estimate of the initial critical height was close to experiment and other model results. The variation of Keff with temperature showed a similar gradient to certain other model results but slightly varied to yet other model results. The calculated control rod worth showed a large difference to other model results. Causes of differences for each test were postulated.

A simplified RZ model was used for this analysis. The FEM method is capable of resolving complex 3D geometries and a more detailed HTR-10 model shown in figure 5.7 was produced. This geometry was constructed using the basic (but flexible) GEM code defining the basic geometry points, lines and regions. The streaming channels in the side reflector are resolved in this model which would give a theoretical improvement over the use of correction factors. To capture the streaming of neutrons in these regions would require transport theory due to the expected anisotropic nature of the flux. The cone region under the active core is not accurately represented but it would be possible in general to retain the cone shape. This 3D HTR-10 FETCH model was impractical to run as convergence was difficult for the even parity formulation within EVENT. Thus this model would require the use of a first order transport FEM solver such as RADIANT Buchan et al. (2010), or the use of a hybrid formulation combining the Even Parity method with a ray tracing method such as that which used to function in EVENT de Oliveira et al. (2001).

This model geometry however still retains the smeared pebble bed. Other research carried out in AMCG focuses on fluids solid particulates modelling in 3D. This methodology is adaptable to pebble bed reactors with the mesh generation being capable of used in RADIANT. However, with the number of pebbles in a reactor of the order of 100,000 (for a small test reactor) a massively parallel solver would be needed. Resolving the heterogeneity associated with the streaming channels and pebbles may thus be possible in the near future. Removing the heterogeneity of the TRISO particle level deterministically in a whole core model is considered practically impossible with foreseeable future method capabilities. This is because the number of TRISO particles in HTGR’s can go into the billions.
Figure 5.7: HTR-10 3D FETCH geometry model resolving the reflector streaming channels (which are control and coolant inlet channels). The colours represent different materials. Meshless regions are those that would contain pure gas.
5.3. Generic Prismatic Block Type Very High Temperature Reactor

The prismatic Very High Temperature Reactor, VHTR(pr), design considered herein is based on the Russian (in collaboration with General Atomics) Gas Turbine-Modular Helium Reactor (GT-MHR) by P. and LaBar (2002). The GT-MHR is itself based on many years of research including the demonstration Fort St. Vrain high temperature reactor and the prototype DRAGON reactor. This provides an encouraging and sound basis for the development of a VHTR(pr), as many of the core components will have been suitably chosen and optimised for an albeit similar reactor with similar generic aims.

Two significant differences between the GT-MHR and the VHTR(pr) exist for the VHTR(pr) to adhere to the specific requirements of the Generation IV project. Firstly the GT-MHR is being designed to utilise weapons grade plutonium as a fuel source, where as for sustainable and commercial reasons the VHTR(pr) is envisioned to be capable of various fuel cycles. Initially the VHTR(pr) will be based on a uranium fuel cycle with a high burnup up for maximum fuel utilisation. However other possibilities will be investigated including the use of fertile thorium, Mixed Oxide fuel (MOX) and for the incineration of other minor actinide’s. The second difference concerns the helium coolant inlet/outlet conditions. The GT-MHR will operate with inlet and outlet coolant temperatures of 490 °C and 850 °C respectively. For the application of process heat (for industrial uses such as hydrogen production) the VHTR(pr) will have an average outlet coolant temperature of 1000 °C, with a corresponding inlet coolant temperature of around 500 °C. The main core layout, constructed of hexagonal graphite blocks in an annular configuration, is presumed identical to the GT-MHR. The GT-MHR and the VHTR(pr) both have an operating power of 600MWt. For the VHTR(pr) to achieve a higher coolant outlet temperature, the mass flow term in the energy balance (an enthalpy balance is not required as helium remains single phase gas under all core conditions) must be altered to remain at the same core power as the GT-MHR. A simple core energy balance requires that the heat energy produced in the fuel must equal the heat energy gained by the coolant as it progresses through the core. To state this mathematically the
coolant mass flow rate, $\dot{m}$, is first defined as

$$\dot{m} = \rho v A \quad (5.3)$$

where $\rho$ is the coolant density, $v$ the coolant speed and $A$ the cross sectional area through which the coolant flows (i.e. the area of a pipe). The core energy balance can then be stated as

$$\dot{m}c_p\Delta T = P \quad (5.4)$$

where $c_p$ is the specific heat capacity of the coolant at constant pressure, $\Delta T$ is the mean change in coolant temperature across the core and $P$ is the total core thermal power. One obvious method to increase outlet temperatures would be a corresponding increase for inlet temperatures. The inlet temperature would be determined by the out of core energy conversion cycle and is beyond the scope of this research. However, an increased inlet temperature is undesirable with regard to the steel reactor pressure vessel. Assuming a fixed inlet temperature, it is then obvious that for a specified core power (600MWt) to achieve a higher coolant outlet temperature while maintaining the energy balance the mass flow rate must be reduced. Thus, the VHTR(pr) has a mass flow rate of 230Kg/s compared to 320Kg/s for the GT-MHR. Another method to increase coolant outlet temperatures would be to increase the generated power while retaining the same mass flow rate. For a fixed core geometry (including height) this would imply an increase in power density. However, the power density is controlled via the mass flow rate and limited due to passive heat removal capabilities during an loss of coolant accident. One could also increase the height of the active core for the same total core power, thus decreasing the average power density. For a specified total core height design this could be achieved by a partial withdraw of control rods. This would induce a positive reactivity, disturbing the neutronic balance causing increased fission reaction rates, which is then compensated by an increase in core temperature that then induces negative reactivity until balance is restored. However, this would shorten the length of an individual fuel cycle as the required active core approaches the total core height sooner. Therefore the best option to increase the outlet temperature is to reduce the mass flow rate, as specified in the VHTR(pr) design.
In the next subsection the design of the VHTR(pr) is described. This design was obtained through an agreement with the company AMEC and is part of an international IAEA coordinated research benchmark that is yet to be published.

5.3.1. VHTR(pr) Design

The VHTR(pr) will have a power of 600MWt with an helium coolant inlet/outlet temperature of 500/1000°C. The helium coolant will be at a pressure of 70bar and have a core mass flow rate of 230Kg/s. The core is constructed from prismatic graphite blocks (with fuel, burnable poison, coolant and control insertions where appropriate) with a cross width of 36cm, a height of 80cm and a density of 1.73g/cc with an equivalent impurity of 1.1ppm of natural boron. The active core height is 800cm corresponding to block stacks 10 high with no vertical gap between each. The blocks are arranged to form an annular core with an inner reflector, central fuel annulus and then outer reflector. The inter-block gap is assumed to be 0.25cm between opposing faces (although this would change with thermal expansion and irradiation). The inner reflector consists of 5 rings (including the centre block as a ring) containing 61 graphite blocks. There are then 3 fuel rings consisting of 30, 36 and 36 fuel blocks respectively (6 blocks in third fuel ring are not fuelled). Surrounding the fuel annulus is then a further 102 reflector blocks. Non-hexagonal blocks are then used to adhere to the cylindrical shape of the pressure vessel, thus extending the outer reflector to a diameter of 700cm. Above and below the core the reflector is formed from a layer of 80cm blocks and a layer of 50cm blocks giving a reflector axial length of 1060cm.

The fuel blocks come in two types depending on whether there is a control channel or not. Type 1 fuel blocks have 108 coolant channels, 216 fuel holes and no control channel. The coolant holes have a diameter of 1.6cm and the fuel hole a diameter of 1.27cm. Coolant channels are distributed fairly evenly over the block (apart from the centre which contains a block handling hole which is assumed filled with graphite due to unknown dimensions) with fuel holes positioned at the corners of a hexagon that is centred on the coolant channel (except at edges). The pitch between any type of channel/hole is 1.9cm. Type 2 fuel blocks have 89 coolant channels (with same diameter
as Type 1) and 174 fuel holes (also same diameter as Type 1) arranged in a similar pattern as Type 1. However, Type 2 fuel blocks contain one control channel with diameter 13cm (hence the reduction in coolant and fuel). Within the core there are 72 stacks of Type 1 fuel blocks and 30 stacks of Type 2, totalling 102 fuel stacks. A planar view of the core showing the annular arrangement is shown in figure 5.8.

Every coolant channel and control channel run the full length of the residing block. Fuel holes stop short of the bottom of the block by 2.5cm and have a 2cm graphite plug at the top. Each fuel hole contains 15 fuel compact inserts of 5cm length and diameter 1.25cm. This leaves a gap of 0.5cm high above the fuel in each channel and a slight radial gap of 0.01cm between the fuel compact and graphite for thermal expansion. Certain radial reflector blocks also contain a control channel of diameter 13cm and are positioned in the outer reflector. Axial reflector blocks continue to have the same number of coolant holes as the type of fuel block in their stack, as well as a control channel if required. All the reflector blocks in the outer-most ring of the inner reflector (24 stacks) within the active core height have six burnable
poison channels of the same structure as fuel channels. Within these channels 15 burnable poison compacts of the same dimensions as fuel compacts are placed. These six burnable poison channels are located in the corners of the hexagonal block in the XY plane. The general layout of the core is observed to be extremely similar to the GT-MHR design.

Within each fuel compact 2493 TRISO particles are distributed. A TRISO particle consists of a Uranium Dioxide ($UO_2$) spherical kernel with an enrichment of 14% U235, a diameter of 0.05cm and a density of 10.2g/cc. This kernel is then surrounded by a carbon buffer layer of thickness 0.0095cm and density 1.0g/cc. There are then three ("TRI") layers comprised of pyrolytic carbon, silicon carbide and pyrolytic carbon again. These have densities of 1.8/3.2/1.8g/cc and a thickness of 0.004/0.0035/0.004cm respectively. This gives a TRISO particle diameter of 0.092cm and a packing fraction (or volume fraction) of TRISO particles within a fuel compact of 0.165655. TRISO particles are the same as that used in the PBMR program but with a different enrichment.

Within the whole core there are 3115800 fuel compacts producing an initial core loading of 4570Kg of LEU. The GT-MHR core contained burnable poison within the fuel blocks in place of fuel compacts. The burnable poison, made from Erbium, is required in the GT-MHR to ensure a negative temperature coefficient of reactivity for a fully plutonium loaded core. Because the VHTR-pr is initially aimed at a uranium fuel cycle these erbium burnable poisons were deemed unnecessary and replaced with fuel compacts.

The VHTR(pr) has 4 movable control systems. There are 12 start up control rods located within the inner most fuel ring. These control rods are inserted into the control channels of Type 2 fuel blocks. There are then 36 control rods arranged around the inner most ring of the outer reflector that are inserted into graphite reflector blocks. These have two purposes, 33 are used to compensate for the reactivity loss due to burnup (fuel depletion and fission product poisoning) and 3 are used for automatic control. When the control rods are fully inserted they extend the full length of the active core as well as the upper axial reflector (i.e. a length of 930cm). Control rods are constructed from a series of 4 annuli, three of which are graphite with density 1.73g/cc and one of boron carbide ($B_4C$). Within the fuel annulus there are an additional 18 control channels for the insertion of emergency boron balls. These have a diameter of 0.6cm and a density of 1.3g/cc natural
When inserted they are assumed to have a packing fraction of 0.6 and can fill from the bottom of the active core to the top (i.e. a height of 800cm).

In the analysis that follows the control rods and boron balls that are inserted into the active fuel regions (type 2 fuel assemblies) are not considered. Further mention of control rods refers solely to the control rods inserted into the outer reflector.

5.4. VHTR MONK Model

In this section the range of MONK9 ANSWERS-MONK VHTR models constructed are described and results presented. The models cover the range from an infinite lattice of TRISO particles to the whole core VHTR including the control rods and burnable poisons. Results are presented for the criticality factor at one temperature of 293 Kelvin. The continuous (13,193 fine groups) JEF2 based DICE library was used for all results. Details considering the treatment of thermal scattering and resonances are described in more detail in the manual ANSWERS-MONK.

MONK9 is an established Monte Carlo based code with extensive verification and validation evidence. Efficiency of modelling (setting up and running) is achieved through the use of Woodcock Tracking and Superhistories. Woodcock Tracking uses the largest total cross section (hence shortest mean free path) for a neutral particle interaction within a region that may contain multiple materials. This is then used to track and tally the particle through this region. This alleviates the need to calculate the distance between geometric bodies (which is called Fractal Geometry tracking) and only needs a rapid algorithm to deduce the material properties at a particular location. Using the shortest mean free path will result in extra collisions that are called virtual collisions. An algorithm is used to determine whether a collision is virtual or real so as to know when to tally a result. Superhistories entails tracking the progeny neutrons produced from fission for a certain number of generations (usually 10) for each neutron initiated within each stage (or batch). This aids in reducing statistical bias in the sampled results and concentrates results on the most reactive parts of the system.

The Monte Carlo method is used extensively and universally for reactor analysis. It is considered the most accurate method and can be thought of as an accurate simulation of reality. Complexity in geometric modelling capabil-
ity is limited by the model and users capability, in theory any geometry can be used. Thus with as accurate a geometry as required the accuracy is determined by the statistical sampling and the material data libraries. Errors (as opposed to accuracy) are also possible due to code and user malfunction but can be reduced through rigorous Quality Assurance processes. Data libraries used in Monte Carlo models (as well as deterministic) are generally international projects such as JEF, ENDF and JENDL. These themselves are constantly maintained, reviewed and improved as appropriate.

Both the MCNP and MONK codes have been used for HTGR analysis. MCNP is used for the design studies of the NGNP reactor MacDonald and et al. (2004) MacDonald and et al. (2003). MONK has been used extensively for pebble bed reactor analysis and recently comparisons where made between MONK9 and MCNP (4.5 and X2.5) for a block type plutonium fuelled VHTR type reactor Zakova and Talamo (2008). Comparisons showed around a 500pcm difference for the criticality factor which where attributed to differences in the geometric modelling, data library, delayed neutron inclusion or not and energy group structure. Around a 500pcm difference was reported between the use of a regular TRISO lattice and a random TRISO lattice. This was attributed to the clipping of TRISO particles for the regular lattice and the average TRISO particle pitch. MCNP was used by multiple participants of the HTR-10 (and HTTR) IAEA-TECDOC-1382 (2003) validation benchmark discussed in a previous section. The results showed that MCNP (plus the Monte Carlo method it represents) model is capable of accurately predicting the core $K_{eff}$ and control rod worth.

The primary purpose of the MONK9 VHTR models constructed were to function as a cross comparison with the WIMS9-FETCH models. The MONK9 models are considered more accurate than the WIMS9-FETCH models and are taken as a reference. The whole core integral $K_{eff}$ factor is used for comparison only. Fluxes could be compared but was not possible during the time available to perform this research. Future versions of MONK will include the ability to have a sampling mesh specified separate from the geometry input. This sampling mesh could be taken directly as the FETCH mesh to give an efficient method for comparison between the models. The TRISO particles in the VHTR MONK9 model produced are on a regular lattice rather than a random lattice. The latter is only possible currently in development versions of MONK for pebble bed geometries. Considering
this and the differences between models used in the HTR-10 and HTTR benchmarks an agreement between MONK9 and WIMS9-FETCH within 1% will be considered good.

The Keff (or $K_\infty$) results presented are the cumulative K-Three values of the MONK9 output. Sufficient settling stages are used to obtain an accurate fission source distribution and sampling stages are run to different accuracies with regard to statistical standard deviations. The initial source distribution was defined to be within all the fuelled regions (being the TRISO kernels) for all simulations.

Figure 5.9 shows the geometry used to model a single TRISO particle in a box with all reflect boundary conditions. This infinite cubic lattice is used as the first comparison with WIMS9. The $K_\infty$ calculated was 1.2316178 with a standard deviation of 0.00295792.

Figure 5.10 shows the geometry used to model the repeat unit cell approximation of fuel assembly type 1. This is effectively a mimic of the geometry used in the WIMS9 model and has an approximate curved outer boundary that uses the white reflective condition. The top and bottom boundary condition is reflective. The TRISO particles are on a regular tetrahedral close packed lattice and can be seen to be clipped by the edge of the fuel compact. The axial heterogeneity is accounted for by an increase in the moderator and coolant radii. The $K_\infty$ calculated was 1.62658348 with a standard deviation of 0.00298029.

A MONK9 model representing fuel assembly type 1 in geometric detail in the XY plane but without accounting for the axial heterogeneity gave a $K_\infty$ of 1.59741137 with a standard deviation of 0.00298455. This model is referred to as the modified fuel assembly 1 model and is useful as a comparison to WIMS9 CACTUS models. Note that this result is not comparable to the previous or the following as the axial heterogeneity is not accounted for which results in a different ratio of fuel to moderator.

Figures 5.11 and 5.12 show the geometry used to model fuel assembly type 1 (FA1). Reflect boundary conditions on the top and bottom and periodic on the six hexagonal sides are used to give an infinite array of assemblies. Axial heterogeneity is accounted for in this model. The $K_\infty$ calculated was 1.61664923 with a standard deviation of 0.00297930. The relative difference between this more accurate model and the unit cell model is 614.5pcm which can only be attributed to the use of a white boundary condition and axial
Figure 5.9.: MONK9 model of TRISO unit cell in a cube.
Figure 5.10.: MONK9 model of fuel compact unit cell with approximate curved outer boundary for comparison with WIMS9.
Figure 5.11.: MONK9 model of fuel assembly type 1 using a regular lattice for TRISO particles.
Figure 5.12: MONK9 model of fuel assembly type 1 shown in an XY cut plane using a regular lattice for TRISO particles.
Figure 5.13: MONK9 model of fuel assembly type 2 using a regular lattice for TRISO particles.
Figure 5.14.: MONK9 model of the geometry of a reflector block with a control rod inserted shown using an XY cut plane.
Figure 5.15.: MONK9 model of the geometry of a reflector block with burnable poisons inserted shown using an XY cut plane.
Figure 5.16.: MONK9 model of the whole core VHTR shown in 3D with a brick cut away to show the internal core.
Figure 5.17.: MONK9 model of the whole core VHTR with control rods inserted and burnable poisons shown using an XY cut plane.
approximation of the latter.

Figure 5.13 shows the geometry used to model fuel assembly type 2 (FA2). Again, reflect boundary conditions on the top and bottom and periodic on the six hexagonal sides are used to give an infinite array of assemblies. Also, axial heterogeneity is accounted for in this model. The $K_{\infty}$ calculated was 1.63934937 with a standard deviation of 0.00294154. This is larger than the $K_{\infty}$ of fuel assembly 1 as the moderator to fuel ratio is larger for fuel assembly 2 and they are both under moderated.

Figure 5.14 shows the geometry used to model the control rod inserted into a reflector block. The control rod model used has already had any axial heterogeneity smeared. Figure 5.15 shows the geometry used to model the outermost ring of inner reflector blocks with burnable poison inserts. Axial heterogeneity is represented in that the burnable poison inserts extended 75cm of a 80cm reflector block (like a fuel insert).

Fuel assembly type 1 and type 2 blocks are stacked 10 high and then a top and bottom reflector of 130cm (80cm block plus 50cm block) added to both to form fuel assembly type 1 and 2 stacks. Coolant and control channel holes
are included in the top and bottom reflector blocks as needed. Also each stack has associated with it half the inter hexagonal block gap. Similarly the reflector blocks are stacked and where needed the burnable poison and control rod channel (with and without rod) blocks used. The burnable poison reflector blocks extend axially the active core zone. The control rod channel blocks extend through the entire axial domain and control rods are inserted from the top of the model domain to the bottom of the active core height when fully inserted.

The 3D whole core MONK9 model is shown in figures 5.16, 5.17 and 5.18. Simulations were performed for the whole core with no control rods and no burnable poisons first. The Keff calculated was 1.50525831 with a standard deviation of 0.00099514. The fraction of neutrons leaking from the core was calculated as 2.94%. The fraction of total neutron absorptions in the fuel was calculated as 89.7% with the rest absorbed in the boron impurities of the graphite. Of these absorptions in the fuel 21.61% were in the resonance energy range.

Including the burnable poisons in the inner reflector blocks reduced the calculated Keff to 1.39809633 with a standard deviation of 0.00099666. The fraction of neutrons being absorbed in the fuel was reduced to 84.76% implying about 5% are absorbed in the burnable poisons. The fraction of neutrons leaking increased slightly to 3.49%. The burnable poison worth (BPW) calculated from

\[
BPW = \left( \frac{1}{K_{\text{eff}}^{BP_{\text{in}}}} - \frac{1}{K_{\text{eff}}^{BP_{\text{out}}}} \right) \times 100
\]  

(5.5)

is thus 5.092%.

Including all the control rods in the outer reflector to fully inserted further reduced the Keff to 1.19243690 with a standard deviation of 0.00009997. This has a standard deviation an order of magnitude lower than previous runs and required around 10 million superhistories and 100 million samples (or neutrons) tracked. The fraction of neutrons absorbed in the fuel was reduced to 73.04% implying that about 12% are absorbed in the reflector control rods. The control rod worth is deduced to be 12.34%. The fraction of neutrons leaking from the domain was reduced to 1.118% possible due to the reflector control rods.

A summary of the MONK9 model results for the original VHTR design
at 293 Kelvin is shown in table 5.6.

<table>
<thead>
<tr>
<th>MONK9 Model</th>
<th>Keff or $K_\infty$</th>
<th>Standard Deviation</th>
</tr>
</thead>
<tbody>
<tr>
<td>TRISO Box</td>
<td>1.23161678</td>
<td>0.00295792</td>
</tr>
<tr>
<td>FA1 Unit Cell</td>
<td>1.62658348</td>
<td>0.00298029</td>
</tr>
<tr>
<td>FA1 Modified</td>
<td>1.59741137</td>
<td>0.00298455</td>
</tr>
<tr>
<td>FA1</td>
<td>1.61664923</td>
<td>0.00297930</td>
</tr>
<tr>
<td>FA2</td>
<td>1.63934937</td>
<td>0.00294154</td>
</tr>
<tr>
<td>VHTR no CR no BP</td>
<td>1.50525831</td>
<td>0.00099514</td>
</tr>
<tr>
<td>VHTR no CR</td>
<td>1.39809633</td>
<td>0.00099666</td>
</tr>
<tr>
<td>VHTR</td>
<td>1.19243690</td>
<td>0.00099977</td>
</tr>
</tbody>
</table>

Table 5.6.: Summary of the MONK9 model VHTR results for the original design at 293 Kelvin.

It is observed that the Keff for the whole core VHTR with control rods and burnable poisons inserted is too high with an excess reactivity of 16.14% or 24.8$\$ (using a 1$ of 0.0065). The temperature increase of the reactor at full power operation is not expected to be able to compensate for this amount of excess reactivity. Therefore the design was varied in the simplest possible way via lowering the fuel U235 enrichment from 14% to 6% in 2% intervals. MONK9 calculations of the whole core with burnable poisons and control rods inserted for these varying enrichments are shown in table 5.7.

<table>
<thead>
<tr>
<th>Enrich.</th>
<th>Keff</th>
<th>St. Dev.</th>
<th>F. A. F. (%)</th>
<th>F. A. R. (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>1.19243690</td>
<td>0.000009997</td>
<td>73.04</td>
<td>30.72</td>
</tr>
<tr>
<td>12</td>
<td>1.16769749</td>
<td>0.00016101</td>
<td>72.09</td>
<td>29.72</td>
</tr>
<tr>
<td>10</td>
<td>1.13606805</td>
<td>0.00016355</td>
<td>70.90</td>
<td>28.69</td>
</tr>
<tr>
<td>8</td>
<td>1.09145630</td>
<td>0.00016461</td>
<td>69.21</td>
<td>27.62</td>
</tr>
<tr>
<td>6</td>
<td>1.02637036</td>
<td>0.00016687</td>
<td>66.78</td>
<td>26.52</td>
</tr>
</tbody>
</table>

Table 5.7.: Summary of the MONK9 model VHTR results for varying U235 enrichment with control rods and burnable poisons inserted at 293 Kelvin. Enrich. is shorthand for enrichment, St. Dev. is short hand for standard deviation, F. A. F. is short hand for fraction of neutrons absorbed in the fuel and F. A. R. is short hand for fraction of neutrons absorbed in resonance energy range that are absorbed in the fuel.

The presented MONK9 results will be used for comparison with the WIMS9-FETCH model in the following sections.
5.5. VHTR WIMS Model

In this section the range of WIMS9 ANSWERS-WIMS VHTR models constructed for the generation of homogenised cross sections are described and the results presented. Comparisons where possible are made to the MONK9 results of the previous section. Comparisons are made solely using the criticality eigenvalue. Number densities were directly entered into both the MONK9 and WIMS9 input files for each isotope apart from the Oxygen in the fuel kernel. In the MONK9 input this was specified as O16 whereas in the WIMS9 input O was specified which therefore may include O17 and O18 in natural abundances (which are very minimal anyway). The WIMS9 172 fine group cross sections are formed from the same JEF2 library that was used for the MONK9 calculations. All models and results should be assumed to be using the original 14% enrichment unless stated. Tolerances used in the WIMS9 calculations should be assumed to be $1.0E-06$ unless stated.

A simple 1D model of a TRISO particle surrounded by fuel compact graphite was constructed using the WIMS9 modules HEAD - FLURIG - PIP. The spherical geometry is represented in the HEAD input as shells. HEAD interpolates the fine group cross sections for 293 Kelvin and uses Equivalence Theory to perform the resonance self shielding. The FLURIG module calculates the collision probabilities in spherical geometry using a white boundary condition. PIP then solves the 172 group problem using the collision probabilities to give a eigenvalue and eigenvector. The $K_\infty$ was calculated to be 1.233667.

Another model to represent the same geometry was constructed using the WIMS9 modules HEAD - PRES - PROC - RES - PIP. The same spherical geometry was used in HEAD as before. The keyword NORESONANCE was included in HEAD to stop the Equivalence self shielding calculation. Instead sub group resonance self shielding was used for the isotopes U235 and U238 using PRES and RES. The 2D geometry used in PROC was that of a fuel compact embedded with TRISO particles with a white boundary condition. After the sub group self shielding PIP solves as before. The $K_\infty$ was calculated to be 1.231240.

The previous two WIMS9 models of an infinite array of TRISO particles surrounded by compact graphite are comparable to each other and the
MONK9 model of a TRISO particle in a box. These results are presented together in table 5.8. Both WIMS9 models are within one standard deviation of the MONK9 model. The absolute difference between the two WIMS9 models is 2.427E − 3.

To flux homogenise the fuel assemblies a representative geometry in WIMS9 of a unit cell geometry centred on one fuel compact is used. This triangular repeat unit cell prevails through most of both fuel assembly types in the XY plane. To model the TRISO particles the PROC module must be used. The geometry in PROC is restricted to concentric annuli or shells with embedded particles in regions. The triangle unit cell is thus approximated as concentric annuli with a white boundary condition. Considering fuel assembly type 1, FA1, (no control rod channel hole) the axial heterogeneity (being that fuel compacts extend 75cm of the 80cm high fuel assembly) is taken into account via increasing the graphite moderator density in the unit cell model. This effectively moves the graphite from the top and bottom of the fuel assembly to the middle where the fuel is axially present. On the final smear the number densities are then reduced by a factor of 0.9375 (being 75 divided by 80) so as to obtain the correct mass. Resonance self shielding is modelled via the modules HEAD - PRES - PROC - RES - PIP using the sub group approach for the isotopes U235 and U238.

To obtain flux homogenised cross sections for fuel assembly type 2, FA2, (with control channel) an infinite array of modified unit cells is not considered appropriate. FA2 is considered to be two thirds of a FA1 unit cell plus one third of an appropriately volume factored weighted flux smearing of FA1 unit cell. To form the RZ fuel ring materials appropriate smearing of the FA1 and FA2 materials are used. Also a whole smeared fuel ring material is produced within WIMS9 to be used as a driver material for homogenising the other materials (reflector, control rods and burnable poisons).

<table>
<thead>
<tr>
<th>Model</th>
<th>$K_{\infty}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MONK9 TRISO Box</td>
<td>1.231617 (std 0.003)</td>
</tr>
<tr>
<td>WIMS9 FLURIG</td>
<td>1.233667</td>
</tr>
<tr>
<td>WIMS9 PROC</td>
<td>1.231240</td>
</tr>
</tbody>
</table>

Table 5.8.: MONK9 and WIMS9 results of infinite array of TRISO particles surrounded by compact graphite.
The $K_\infty$ results from the two MONK9 models of FA1 (one exact and the other a unit cell similar to the WIMS9 model) and the WIMS9 PROC model of the FA1 unit cell at 293 Kelvin are shown in table 5.9. Close agreement between the exact MONK9 FA1 model and the approximate WIMS9 unit cell model with an absolute difference of $1.699E - 03$ is observed, which is within one standard deviation of the MONK9 result.

To model the TRISO particles embedded within the fuel compacts in WIMS9 only the PROC module is applicable. This allows a homogenised fuel compact material to be produced. Using the spatially smeared fuel compact (retaining 172 groups) a CACTUS model of a modified FA1 in the XY plane was constructed. This is shown in figure 5.19 where one sixth symmetry is exploited with periodic boundary conditions. To deduce whether a more detailed FA1 model was needed the CACTUS result is compared to the unit cell PROC and MONK9 results. This comparison did not take account of axial heterogeneity so is a modified FA1 comparison. Results are shown in table 5.10. The WIMS9 results are within 2 standard deviations of the MONK9 result. The absolute difference between the two WIMS9 models is $3.39E - 04$ and the relative difference being about 20pcm. The use of a more detailed 2D CACTUS fuel assembly model after the fuel compact unit cell model is thus not required. The small difference between the two

<table>
<thead>
<tr>
<th>Model</th>
<th>$K_\infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MONK9 FA1</td>
<td>1.61664923 (std 0.00297930)</td>
</tr>
<tr>
<td>MONK9 FA1 Unit Cell</td>
<td>1.62658348 (std 0.00298029)</td>
</tr>
<tr>
<td>WIMS9 PROC Unit Cell</td>
<td>1.618348</td>
</tr>
</tbody>
</table>

Table 5.9.: MONK9 and WIMS9 results of fuel assembly type 1 (FA1) as an infinite array.

<table>
<thead>
<tr>
<th>Model</th>
<th>$K_\infty$</th>
</tr>
</thead>
<tbody>
<tr>
<td>MONK9 FA1</td>
<td>1.59741137 (std 0.00208455)</td>
</tr>
<tr>
<td>WIMS9 PROC Unit Cell</td>
<td>1.602588</td>
</tr>
<tr>
<td>WIMS9 CACTUS FA1</td>
<td>1.602927</td>
</tr>
</tbody>
</table>

Table 5.10.: MONK9 and WIMS9 results of a modified fuel assembly type 1 as an infinite array.
Figure 5.19.: The geometry of the WIMS9 CACTUS modified fuel assembly type 1 model. The slightly larger circles represent coolant holes and the slightly smaller circles represent the spatially smeared fuel compacts. Everything else is graphite moderator apart from the thin lower strip that represents the inter hexagonal gap.
Figure 5.20: The $K_\infty$ variation with temperature of the WIMS9 FA1 unit cell model for the different enrichments.

WIMS9 models can be attributed to the fuel coolant pitch being 1.9cm and the neutron mean free path in graphite being about 2.6cm for a thermal neutron.

Homogenised cross sections for FA1, FA2 and the three fuel rings used in the FETCH RZ model are produced at different temperatures. A data set with all the materials varied at the same temperature is produced for different enrichments of the U235 being 14%, 12%, 10%, 8% and 6%. Also a data set with separate variations of the fuel kernel and graphite (in the compact and moderator) temperature such as to produce a 2D grid cross section variation is produced.

The $K_\infty$ variation with temperature of the WIMS9 FA1 unit cell model for the different enrichments is shown in figure 5.20. From these results the
temperature reactivity coefficient defined as
\[
\frac{\partial \rho}{\partial T} = \frac{\partial \rho}{\partial K} \frac{\partial K}{\partial T} = \frac{1}{K} \frac{\partial K}{\partial T} \approx \frac{1}{K_1 K_2} \frac{K_2 - K_1}{T_2 - T_1}.
\]  
(5.6)
is calculated and presented in table 5.11.

<table>
<thead>
<tr>
<th>U235 Enrich. (%)</th>
<th>Temp. Range (Kelvin)</th>
<th>Temp. Reactivity Coeff.</th>
</tr>
</thead>
<tbody>
<tr>
<td>14</td>
<td>293 - 773</td>
<td>-4.620835E-05</td>
</tr>
<tr>
<td></td>
<td>773 - 1273</td>
<td>-3.300722E-05</td>
</tr>
<tr>
<td></td>
<td>1273 - 1773</td>
<td>-2.461101E-05</td>
</tr>
<tr>
<td>12</td>
<td>293 - 773</td>
<td>-4.789652E-05</td>
</tr>
<tr>
<td></td>
<td>773 - 1273</td>
<td>-3.443031E-05</td>
</tr>
<tr>
<td></td>
<td>1273 - 1773</td>
<td>-2.582911E-05</td>
</tr>
<tr>
<td>10</td>
<td>293 - 773</td>
<td>-4.992072E-05</td>
</tr>
<tr>
<td></td>
<td>773 - 1273</td>
<td>-3.609780E-05</td>
</tr>
<tr>
<td></td>
<td>1273 - 1773</td>
<td>-2.729852E-05</td>
</tr>
<tr>
<td>8</td>
<td>293 - 773</td>
<td>-5.263617E-05</td>
</tr>
<tr>
<td></td>
<td>773 - 1273</td>
<td>-3.818754E-05</td>
</tr>
<tr>
<td></td>
<td>1273 - 1773</td>
<td>-2.923061E-05</td>
</tr>
<tr>
<td>6</td>
<td>293 - 773</td>
<td>-5.656953E-05</td>
</tr>
<tr>
<td></td>
<td>773 - 1273</td>
<td>-4.106293E-05</td>
</tr>
<tr>
<td></td>
<td>1273 - 1773</td>
<td>-3.200041E-05</td>
</tr>
</tbody>
</table>

Table 5.11.: Temperature Reactivity Coefficient for different enrichments of the WIMS9 FA1 unit cell model.

To produce homogenised cross sections for non fuel region materials a 2D annuli whole core model using the WIMS9 module PIJ is used. This consists of three concentric annuli being the inner reflector, fuel ring and outer reflector. A free vacuum boundary condition is used on the outer domain boundary. The fuel region 172 group cross sections are homogenised as needed from the FA1 and FA2 cross sections previously discussed. The RODSUB option in PIJ is then used to place circular arrays on this 2D core model for each geometry of interest. This includes the following:

- Outer/Inner reflector blocks.
• Outer reflector blocks with control rod channel.
• Outer reflector blocks with control rod channel with control rod in.
• Inner reflector blocks with burnable poison inserts.
• Top and bottom reflector blocks that are above and below fuel assemblies type 1 and 2.

Outer reflector blocks with a control rod channel (with and without rod) are produced for being represented in one third of a hexagonal block as this is what is represented within the most detailed FETCH model. This is then used to produce a whole hexagonal homogenised reflector block with control rod in (or out) material, which itself is then used to produce the outer homogenised reflector ring with control rods in (or out) for the RZ FETCH model. No temperature variation is considered for non fuel materials including the reflectors.

All the spatially homogenised materials are collectively energy condensed to a range of number of groups from 172 down to 2 that are decided through energy interval halving as best as possible. The WIMS2BEANS.py python script is then used to process the WIMS9 output into a format suitable for read in to both FETCH-E and FETCH-B. Cross sections used in FETCH-B also have the option to take account of streaming corrections to form anisotropic diffusion coefficients using the Behrens formula discussed previously for the HTR-10 benchmark.

5.6. VHTR FETCH Model

In this section the range of geometric whole core VHTR FETCH models for radiation transport calculations are described. Static eigenvalue results are analysed for spatial, energy and angle convergence. Comparisons are made between the different whole core FETCH models as well as to the MONK9 model where possible. Unless stated the FETCH convergence tolerances should be assumed to be $1.0E-08$. Spatial flux plots use a linear interpolation for the colour scheme even if the solution used quadratic basis functions.

Three whole core FETCH models were produced being one 2D RZ and two 3D XYZ models. The difference between the two 3D XYZ models is
in the geometric material mapping. One uses full homogenised hexagonal blocks while the other allows for the hexagonal block to be divided into three materials. The full homogenised hexagonal block model is referred to as the XYZ whole hexagon model. The model allowing three material thirds within a hexagon is referred to as the XYZ third hexagon model. The RZ model uses a quadrilateral mesh and the XYZ models use a hexahedral mesh. This is because the purpose of these models is to be used also in FLUIDITY for coupled analysis which requires this restriction of element choice. The 2D RZ model represents the fuel assemblies as three annuli that preserve volume. A vacuum boundary condition is used on the outside domain surface of each model.

Figure 5.21 shows the RZ FETCH model with mesh divisions chosen radially and axially to mimic the number of divides of the XYZ models as best as possible. Figure 5.22 shows a XY planar cut of the XYZ whole hexagon FETCH model with the minimum mesh. The axial geometry of this model is constructed through stretching (zoning) the XY geometry shown and changing the materials as required for each zone. Thus an axial planar cut of the XYZ model would look similar to the RZ picture. The XYZ domain can be observed to have a sixth rotational symmetry due to the positioning of the reflector control rods. The outer domain boundary conforms to the cylindrical edge of the reflector design using linear geometric elements. Figure 5.23 shows a XY planar cut of the XYZ third hexagon FETCH model with the minimum mesh.

In the following subsections the spatial, angle and energy convergence is analysed as is the effect of including streaming corrections. The RZ and a 2D XY plane model are analysed to infer conclusions for the full 3D XYZ model with regard to convergence. The RZ and XYZ models are used to analyse the effect of applying streaming corrections. The resulting phase space resolution of the RZ and XYZ models is then used to analyse the VHTR with comparisons to MONK9 model. This includes analysis of the variation of the $K_{\text{eff}}$ with respect to temperature for decreasing enrichments, for the case of all reflector control rods in and including burnable poisons.
Figure 5.21.: The FETCH 2D RZ VHTR model. Colours represent different materials. The mesh is representative of the reference mesh deduced most suitable for the 3D XYZ calculations. The red and two orange colours are the three pseudo fuel rings with the central z axis on the left side.
Figure 5.22: The FETCH 3D XYZ VHTR whole hexagon model shown via a XY planar cut. Colours represent different materials. The mesh shown is the minimum in the XY plane needed to define the geometry of the third hexagon model. Red is FA1, orange is FA2, blue is outer reflector with control rod, green the inner reflector with burnable poison and pale green reflector blocks.
Figure 5.23.: The FETCH 3D XYZ VHTR third hexagon model shown via a XY planar cut. Colours represent different materials. The mesh shown is the minimum in the XY plane needed to define the geometry. Red is FA1 (or part of FA2), orange is the third part of FA2, blue is outer reflector with control rod, green the inner reflector with burnable poison and pale green reflector blocks.
5.6.1. Spatial Convergence

The mesh convergence of the 2 group problem in RZ geometry with control rods in and burnable poisons is first analysed. Transport cross sections with streaming corrections applied are used within BEANS. Both linear and quadratic basis functions are used. The Keff is used as a measure of accuracy. The temperature of all materials is 293 Kelvin. The coarsest mesh is that shown in figure 5.21 which has 408 elements. The reference mesh solution is the coarsest divided in each axis by 8 to give 26112 elements and 105185 nodes using quadratic basis functions. The mesh with 1632 volume elements is the coarsest divided in each axis by 2 and the mesh with 6528 volume elements is the coarsest divided in each axis by 4. Results are shown in table 5.12. The coarsest mesh solution using quadratic basis functions has a relative error of just under 11pcm. This favourable result is highlighted as this is the mesh that will be used for the coupled simulations. The two group fluxes and the power density for the 408 element quadratic solution are shown in figures 5.24, 5.25 and 5.26. The flux has been normalised to the design power of 600MW. Using isothermal conditions with no thermal feedback the spatial flux and power density solutions are practically symmetric about the Z axis centre of the active core. The fast and thermal fluxes show characteristic behaviours. The average power density was calculated as 6.4612W/cc, the maximum power density as 10.2395W/cc and hence the power peaking factor as 1.5848.

The axial mesh resolution used for the RZ model is inferred to be ap-

<table>
<thead>
<tr>
<th>Volume Elements</th>
<th>Basis Order</th>
<th>Keff</th>
<th>Rel. Keff Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>408</td>
<td>linear</td>
<td>1.24658</td>
<td>8.9347E-04</td>
</tr>
<tr>
<td>1632</td>
<td>linear</td>
<td>1.24746</td>
<td>1.8787E-04</td>
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<tr>
<td>6528</td>
<td>linear</td>
<td>1.24764</td>
<td>4.1802E-05</td>
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<tr>
<td>26112</td>
<td>linear</td>
<td>1.24768</td>
<td>1.0026E-05</td>
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<tr>
<td>408</td>
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<tr>
<td>26112</td>
<td>quadratic</td>
<td>1.24769</td>
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Table 5.12.: Mesh convergence of the Keff for the RZ 2 group FETCH VHTR model using linear and quadratic basis functions. The reference solution is taken as the finest quadratic solution.
Figure 5.24.: The group 1 (fast flux) solution of the 2 group RZ FETCH VHTR model using 408 elements with quadratic basis functions. The flux density has been normalised to the design power of 600MW.
Figure 5.25.: The group 2 (thermal flux) solution of the 2 group RZ FETCH VHTR model using 408 elements with quadratic basis functions. The flux has been normalised to the design power of 600MW.
Figure 5.26.: The element wise power density of the 2 group RZ FETCH VHTR model using 408 elements with quadratic basis functions. The units of the power density are W/cc.
appropriate for the axial mesh resolution of the 3D XYZ model also as they both have the same axial material detail. To analyse the mesh resolution in the XY plane of the XYZ model a series of calculations refining the mesh using a 2D XY plane model only is used. This XY plane model is a slice through the active core height and corresponds to the geometries shown in figures 5.22 and 5.23. Linear and quadratic basis functions are compared. The coarsest mesh is that shown in figures 5.22 and 5.23 to define the geometry using quadrilaterals in 2D. Finer meshes involve dividing every line shown equally into a number of intervals. Again the materials were all at 293 Kelvin and the Keff is used as an error measure. The reference answer uses quadratic basis functions with 5 line divides to give 45450 elements. The whole hexagon and third hexagon geometries are analysed. Results are shown in tables 5.13 and 5.14. The superiority of using quadratic basis

<table>
<thead>
<tr>
<th>Volume Elements</th>
<th>Basis Order</th>
<th>Keff</th>
<th>Rel. Keff Error</th>
</tr>
</thead>
<tbody>
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<tr>
<td>7272</td>
<td>linear</td>
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<td>linear</td>
<td>1.22924</td>
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</tr>
<tr>
<td>45450</td>
<td>quadratic</td>
<td>1.22978</td>
<td>0.0</td>
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</table>

Table 5.13.: Mesh convergence of the Keff for the 2D XY whole hexagon 2 group FETCH VHTR model using linear and quadratic basis functions. The reference solution is taken as the finest quadratic solution.

functions over linear is evident. For the coarsest mesh (1818 elements) the quadratic solution for the whole hexagon model has a relative error of 8pcm and for the third hexagon model has a relative error of 14pcm. To achieve this accuracy with linear elements would require more than 45450 elements for both these 2D cases and this would be a severely impractical mesh to use in a 3D coupled analysis. Also the CPU time taken for the quadratic 1818 element simulations were 10 times smaller than the CPU times of the finest linear 45450 element simulations, which still had an error twice as large in
<table>
<thead>
<tr>
<th>Volume Elements</th>
<th>Basis Order</th>
<th>Keff</th>
<th>Rel. Keff Error</th>
</tr>
</thead>
<tbody>
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<td>1.18021</td>
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<td>1.18982</td>
<td>2.82764E-03</td>
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<td>16362</td>
<td>linear</td>
<td>1.19167</td>
<td>1.27821E-03</td>
</tr>
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Table 5.14.: Mesh convergence of the Keff for the 2D XY third hexagon 2 group FETCH VHTR model using linear and quadratic basis functions. The reference solution is taken as the finest quadratic solution.

The coarsest quadratic mesh is concluded to be sufficiently accurate and the most computationally efficient mesh. This quadratic mesh is taken as a converged mesh for the XYZ models. However for coupled analysis the same mesh but using linear basis functions will also be used for the XYZ models as it is computationally faster but must be recognised to be not spatially resolved.

The 2D XY plane third hexagon 2 group VHTR problem was also analysed using the Sub Grid Scale (SGS) method developed in the preceding chapter 4. The original SGS method using linear basis functions for both the global and fine scales was compared to the use of the standard Continuous Galerkin (CG) method using linear and quadratic basis functions. The error convergence (using the finest CG quadratic as the reference) of each method is compared in figure 5.27. The l-l SGO method can be seen to be superior to the linear CG method consistently reducing the error for each mesh resolution by just over a half. The l-q SGO method performed no better than the l-l SGO method for this case and so cannot be used in place of the quadratic CG method.
Figure 5.27.: The relative $K_{eff}$ error of the SGS original method using linear basis functions on both scales compared to standard CG method for the 2D XY plane VHTR model using 2 energy groups.
5.6.2. Angular Convergence

To analyse the angular convergence of the whole core model geometries the RZ and XY third hexagon plane 2 group models where used in both EVENT and BEANS. No streaming corrections were applied for this analysis. Again the materials were at a temperature of 293 Kelvin and the Keff is used for comparison. The RZ model used 408 linear elements which was previously shown to have a spatial error of about 90pcm for diffusion theory. The XY model used 45450 linear elements which was previously shown to have a spatial error of about 47pcm for diffusion theory. The results of varying the flux angular and scatter expansion are presented in table 5.15 for the RZ model and in table 5.16 for the XY plane model. The difference between

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Table 5.15.: The Keff for the RZ VHTR EVENT and BEANS models for different angular approximations (flux expansion then scatter kernel expansion where Tr refers to the use of transport cross sections). No streaming corrections are considered and 2 energy groups were used.

EVENT and BEANS for the P1P0 (isotropic scatter diffusion theory) is less than 1pcm as expected for both models. The relative difference between isotropic scatter (P1P0) and linear anisotropic scatter (P1P1) in EVENT is 0.78% for the RZ model and 0.9% for the XY plane model. This is less than what was observed for the HTR-10 FETCH model presented in previous sections where the difference was 2.2%. The HTR-10 core was however much smaller being about 100cm high and with a radius of 90cm whereas the VHTR is over 10 times taller and with a radius of 350cm.
Table 5.16.: The $K_{eff}$ for the XY third hexagon VHTR EVENT and BEANS models for different angular approximations (flux expansion then scatter kernel expansion where $Tr$ refers to the use of transport cross sections). No streaming corrections are considered and 2 energy groups were used.

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The relative difference between the EVENT P1P1 and the more approximate BEANS P1Tr is 1.05% for the RZ model and 1.2% for the XY plane model.

For the RZ model the relative difference between the use of EVENT Pn or SPn angular expansions is practically negligible being of the order of $1.0E-06$. The relative difference between the EVENT P3P1 and P7P1 is also negligible being of the order of $1.0E-07$. The relative difference between the EVENT P1P1 and P3P1 $K_{eff}$ is $51.46\text{pcm}$ which for whole core coupled analysis is considered small enough to be acceptable. The lack of transport effects within the model is due to the amount of homogenisation needed to spatially represent the whole core.

For the XY third hexagon model the relative difference between the EVENT Pn and SPn order 7 $K_{eff}$’s is $20.47\text{pcm}$. The relative difference between the P3P1 and P7P1 is $3.85\text{pcm}$ and between the SP7P1 and SP3P1 is $1.79\text{pcm}$. The EVENT P3P1 is therefore considered converged in angle. The relative difference between the EVENT P3P1 and P1P1 is $160\text{pcm}$. This increase in transport effects of the XY model compared to the RZ model is considered due to the more local confinement of the control rods. However a $160\text{pcm}$ error for whole core coupled analysis is considered acceptable and P1 diffusion theory is thus applicable for this whole core model.
5.6.3. Streaming Correction Effects

The effects of applying Behrens streaming corrections to the transport (or diffusion) coefficients that are used in the BEANS RZ and XYZ third hexagonal block models are shown in Table 5.17. Streaming corrections are applied for the control rod channel and coolant holes in all the parts of the domain that they occur. Note that this not only applies a correction to the axial direction but also the radial (or XY plane) direction. The RZ model results used 408 quadratic elements. The XYZ model used 21816 quadratic elements which had the same axial resolution as the RZ and 1818 elements in the XY plane. Both the RZ and XYZ models used 2 energy groups with all materials at 293 kelvin. Applying the streaming corrections lowers the

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Table 5.17.: The effect on the Keff of the RZ and XYZ third hexagonal 2 group BEANS VHTR models of applying the Behrens streaming correction.

Keff as there is more leakage from the core and the outer boundary. The reduction between the models is similar. The inclusion of the theoretical streaming corrections has a greater effect than increasing the angular flux expansion to capture transport effects. The effect is however less for the VHTR than that calculated for the HTR-10 again due to the larger size of the VHTR.

Note the relative difference between the XYZ Keff and the XY plane Keff for P1Tr using 2 energy groups is 1.48%. This difference between the axially finite and infinite Keff is not overly large as the VHTR active core is 8 metres high with an annulus active thickness of about 0.94 metres.

Also note that the relative difference between the RZ and XYZ models for the Keff is 5.264% with the RZ being the higher of the two.

The two group fluxes and the power density for the 21816 element quadratic XYZ solution are shown in figures 5.28, 5.29 and 5.30. The flux has been normalised to the design power of 600MW. The thermal flux and power density show that 3D effects are being captured that the RZ model would not. This includes an improved representation of the reflector control rod positions,
Figure 5.28: The group 1 (fast flux) solution of the 2 group XYZ third hexagon FETCH VHTR model using 21816 elements with quadratic basis functions. The flux density has been normalised to the design power of 600MW. Planar cuts leave one quarter of the core visible.
Figure 5.29.: The group 2 (thermal flux) solution of the 2 group XYZ third hexagon FETCH VHTR model using 21816 elements with quadratic basis functions. The flux has been normalised to the design power of 600MW. Planar cuts leave one quarter of the core visible.
Figure 5.30.: The element wise power density of the 2 group XYZ third hexagon FETCH VHTR model using 21816 elements with quadratic basis functions. The units of the power density are W/cc. Planar cuts leave one quarter of the core visible.
the reduced power in fuel regions with control rod channels present and the

general structure of the hexagonal geometry causing flux peaks at inner re-

flectors corners. The average power density was calculated as 6.4612W/cc,

the maximum power density as 11.8811W/cc and hence the power peaking

factor as 1.8388. This corresponds to an increase of about 16% to the RZ

model for the maximum power density.

5.6.4. Energy Group Convergence

To analyse the energy group convergence the BEANS RZ and XY plane mod-

els at an isothermal temperature of 293 Kelvin with the previously stated

quadratic basis function meshes are used. The Keff is compared for both

models with the 172 group calculation considered the reference, being the

maximum available using WIMS9 to produce homogenised cross sections.

For the RZ model the maximum power density is also compared where all

the eigenvector flux results are normalised to the design power of 600MW.

CPU times are also presented. The total number of energy groups consid-

ered are 2, 3, 6, 11, 21, 43, 86 and 172. The 2 group structure has the

energy bound at 4eV being the thermal cut off for WIMS9. The 3 group

structure has a thermal (cut off 4eV), resonance (resonance cut off 183KeV

in WIMS9) and a fast group. The 6 group structure has 2 fast groups, 1

resonance and 3 thermal groups. The 11 group structure has 2 fast groups,

3 resonance groups and 6 thermal groups. The 21 group structure has 4 fast

groups, 7 resonance groups and 10 thermal groups. The 86 group structure

was deduced by removing every other group boundary from the 172 group

structure. Similarly, the 43 group structure was deduced by removing every

other group boundary from the 86 group structure.

The Keff, relative Keff error and CPU time for the XY plane model results

are shown in table 5.18. The CPU time is normalised such that the 2 group

simulation takes one unit time. It is observed that increasing the number

decreases the calculated Keff. The 2 group result has just

over a 2% relative error to the 172 group reference. Using the 3 group

structure reduces this error by just over a half to be just less than 1%, at

the expense of an increase in CPU time of 26%. The use of the 3 group

structure over the 2 is therefore advocated. Going from the 3 to 6 energy

group structures reduces the error by only around 10% but increases the
Table 5.18.: The $K_{eff}$, relative $K_{eff}$ error and CPU time for the XY plane model. The CPU time is normalised such that the 2 group simulation takes one unit time.

required CPU time by over 100\% in comparison. The use of the 3 group structure over the 6 is therefore also advocated. Further increases in the number of energy groups show an accelerating increase requirement of CPU time. The 11 groups has less than a 0.5\% error but takes 10 times longer than the 2 groups and just over 3 times longer than the 6 groups. This more demanding time requirement would be problematic for coupled analysis in 3D XYZ, especially for transients. The 3 energy group structure is therefore deduced to be the most appropriate from these results.

The $K_{eff}$, relative $K_{eff}$ error and CPU time for the RZ model results are shown in table 5.19. Again the CPU time is normalised such that the 2 group simulation takes one unit time. Convergence results for the RZ model

Table 5.19.: The $K_{eff}$, relative $K_{eff}$ error and CPU time for the RZ model. The CPU time is normalised such that the 2 group simulation takes one unit time.
with regard to the $K_{eff}$ are similar to that observed for the XY plane model. The normalised CPU times for the intermediate groups are however less for the RZ model than the XY plane model. The 3 energy group structure is therefore deduced again to be the most appropriate from these results.

The maximum power density and relative maximum power density error for the RZ model results are shown in Table 5.20. Contrary to the $K_{eff}$

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Table 5.20.: The maximum power density and relative maximum power density error for the RZ model.

convergence the reduction in relative error of the maximum power density (a local error as opposed to the $K_{eff}$ being a global error) going from 2 groups to 3 is 6.4% (the $K_{eff}$ error reduced by over 50%). A 61.5% reduction in error occurs going from 3 groups to 6 and then about a 50% reduction from 6 to 11 and 11 to 21 groups. Balancing CPU time and accuracy the 6 and 11 group structures are deduced the most appropriate from these results.

From the presented results for energy group convergence of the RZ and XY plane model the 3, 6 and 11 group structures are each deduced suitable for the XYZ model. The 3 group structure though incurs a larger local error of the maximum power density. The 2 group structure is deduced to have too large an error for physical conclusions to be stated, although still suitable for the previous subsections mesh and angle convergence analysis. Use of more than 11 groups is considered too computationally time consuming for practical application to coupled analysis in XYZ geometry. Note that this conclusion concerns the use of flux weighted homogenised cross sections. Improved techniques of homogenisation may reduce the error associated with the few group structures making them more accurate. These techniques include Super Homogenisation (SPH) that will be a feature of WIMS10 (or
5.6.5. Physical Analysis

In this subsection the RZ and XYZ (whole and third hexagonal material mapping) FETCH VHTR models are used for a physical analysis with comparisons to the MONK9 model. The phase space resolution used is deduced from the previous subsections. Transport effects are considered minimal for the whole core homogenised FETCH models such that the P1 (diffusion in steady state) angular approximation is sufficient. Spatial resolution is 408 quadratic elements for the RZ and 21816 quadratic elements for the XYZ (being 1818 in the plane and then the same axial mesh resolution as the RZ). The use of transport cross sections (as opposed to a P1 scatter kernel) is necessary to apply streaming corrections, even though this incurs an error that was quantified for 2 groups. The last two statements (quadratic basis functions and transport cross sections) implies that BEANS is used rather than EVENT. This is because EVENT can not use anisotropic transport cross sections and was observed to have computational speed issues associated with the use of quadratic basis functions. The energy group structures considered herein are 3, 6 and 11.

Comparisons are first made to the MONK9 model for the whole core VHTR with no reflector control rods inserted and no burnable poisons included within the inner reflector. The results are shown in table 5.21. The isothermal core temperature was 293 Kelvin. Little variation exists between the different energy group structures for each FETCH model. Also little variation exists between the different FETCH geometric models. The XYZ third hexagon material mapping model has a relative difference to the MONK9 model of about 0.19-0.3%. The RZ difference is slightly larger being about 0.27-0.65% and the XYZ whole hexagon model slightly lower being about 0.02-0.38%. These results show that the homogenisation methods used to produce the fuel and reflector regions was performed satisfactory with regard to this global error measure.

Next comparisons are made to the MONK9 model for the VHTR model with no control rods inserted but with the burnable poisons included within the inner reflector. The results are shown in table 5.22. As for the previous case little variation exists between the different energy group structures
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Table 5.21.: Comparison of the Keff of the FETCH VHTR models for no control rods in and no burnable poisons included against the MONK9 model at 293 Kelvin. Results for 3, 6 and 11 groups are shown.

and the different geometric FETCH models. The relative differences are also similar in nature to the previous case. These results show that the homogenisation of the inner reflector blocks with the burnable poison was performed satisfactory with regard to this global error measure. Using the definition 5.5 the burnable poison worth for the XYZ third hexagon model using 11 energy groups is calculated as 5.1481%. Correspondingly the burnable poison worth calculated from the MONK9 model is 5.0919%. The relative difference between these two calculated worth’s is 1.1% which is considered good agreement.

Next comparisons are made to the MONK9 model for the VHTR model with the control rods inserted and with the burnable poisons included within the inner reflector. The results are shown in table 5.23. With the inclusion of the reflector control rods into the models the differences have increased by an order of magnitude. The RZ geometry expectedly performs the worst with a 3-3.5% difference to the MONK9 model. The XYZ whole hexagon and RZ models over estimate the Keff whilst the XYZ third hexagon model under estimates it. The XYZ whole hexagon model has a lower relative difference than the XYZ third hexagon model. However the XYZ third hexagon model is considered the most geometric accurate application of the WIMS9-FETCH models and hence the appearance of a smaller difference of the XYZ whole hexagon model is considered a coincidence. The relative
Table 5.22.: Comparison of the Keff of the FETCH VHTR models for no control rods in but with burnable poisons included against the MONK9 model at 293 Kelvin. Results for 3, 6 and 11 groups are shown.

difference of the XYZ third hexagon model ranges from 1.6-2.2%. This difference is considered due to the homogenisation of the control rod materials within WIMS9 because in previous subsections the transport effects of the FETCH model was deduced to be about 1.6E-03. Improved homogenisation methods over standard flux weighting may reduce this difference and would be possible with future versions of WIMS (10 or 11). Using definition 5.2 the total reflector control rod worth for the 3 group XYZ third hexagon FETCH model is calculated as 13.53%. Correspondingly the control rod worth calculated from the MONK9 model is 12.34%. The relative difference between these two calculated worths is 9.6% and is considered the best currently achievable using the current WIMS9-FETCH model.

Also note that the difference between the RZ and XYZ third hexagon models is over 5% for each energy group structure investigated. This difference does not occur when no control rods are considered and is therefore due to the homogenisation method used to represent these regions in each model.

The variation of the RZ and XYZ third hexagonal FETCH VHTR models with different active core isothermal temperatures and different enrichments is shown in figure 5.31. The temperature range is from 293 Kelvin to 3773 Kelvin and the enrichment range from 6% to 14%. These results are for all the normal operation control systems inserted (control rods and burnable

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Figure 5.31.: The variation of $K_{eff}$ with temperature for decreasing enrichments for the RZ and XYZ third hexagon models using 3 energy groups. Reflector control rods are fully inserted and burnable poisons included. The temperature refers to the isothermal core value.
Table 5.23.: Comparison of the $K_{eff}$ of the FETCH VHTR models with control rods in and with burnable poisons included against the MONK9 model at 293 Kelvin. Results for 3, 6 and 11 groups are shown.

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</tr>
</tbody>
</table>

poisons). For the 14% enriched RZ model for criticality to be reached an isothermal core temperature of about 3000K is implied. For the XYZ model the corresponding temperature is about 2000K. This is clearly too high when the helium outlet of the VHTR core is envisioned to be 1273K, with a maximum accident fuel temperature of 1873K regularly accepted. It was for this reason that the enrichment is reduced to lower the excess reactivity of the VHTR design. The 10% enriched XYZ model suggests criticality at about 1000K isothermally. Correspondingly the 8% enriched RZ model suggests criticality at about 1000K, this is due to the higher prediction of $K_{eff}$ of this model implying a lower enrichment. A more rigorous coupled analysis is presented in the next chapter to determine predictions of the maximum temperatures and power peaking factors of the different enrichment designs at steady state.

Other design changes to lower the excess reactivity could be to increase the TRISO packing fraction (being under moderated), increase the TRISO kernel size (being under moderated) or include further burnable poisons such as into the fuel assembly. The latter is part of the plutonium fuelled version of this reactor but is required not for holding down excess reactivity but to ensure a negative temperature coefficient. The latter would also complicate the design and modelling of the VHTR and is thus not a possible option. Increasing the TRISO particle size and packing fraction has a reliance on
an engineering capability and performance that is not known. Lowering the enrichment is known possible and the simplest option to consider and therefore the chosen option. Lowering the enrichment will affect the fuel cycle length such that going too low would not be an economic reactor. However, the design studies for the U.S.A. VHTR (NGNP reactor) concluded that the initial core loading enrichment should be 10% with refuelling fuel assemblies having an enrichment of 12-15% MacDonald and et al. (2003). However this NGNP design had different TRISO particle sizes and packing fractions and no known literature information regarding use of control rods or burnable poisons.

5.7. Conclusions

Initially a WIMS9-FETCH RZ model was presented and used to analyse the IAEA HTR-10 initial criticality benchmark. Close agreement for the the infinite eigenvalue from WIMS9 with other available model results was achieved being within one standard deviation of a Monte Carlo literature result. Agreement where expected between EVENT and BEANS was shown. Due to the small nature of the HTR-10 core the necessity to account for streaming in reflector channels using anisotropic transport coefficients was deduced. This was expected from reviewing the literature benchmark results. Mesh and angle convergence for the HTR-10 model in RZ was analysed and a suitable quadratic spatial resolution deduced. Using 172 energy groups in BEANS the initial core height was calculated to be 2.2% greater than the experiment. This is considered close agreement. The variation of the Keff with temperature was compared to other literature model results and a similar behaviour was observed. The comparison of the control rod worth showed a large difference to other models and reasons for this were postulated. Future possible improvements to the WIMS9-FETCH model were then discussed for the purpose of modelling the HTR-10.

Following this validation and verification test case a range of radiation transport models were produced and used to analyse a generic block type VHTR. A spatially detailed hierarchy of MONK9 models were presented that used a continuous energy spectrum. The main spatial approximation in these models was a structured array of TRISO particles that were clipped at the fuel compact edges. Literature results analysing this approximation were
discussed. The MONK9 model results for the entire reactor at 293 Kelvin were considered a reference for the WIMS9-FETCH models that followed. These comparisons involved solely using the eigenvalue as a global error measure.

A range of different modules in WIMS9 were used to compare to MONK9 with agreement for the fuel assembly model being within one standard deviation of the MONK9 result. The ability to use a more detailed CACTUS model for the fuel assemblies was concluded to be not needed. A description of the modules and inputs used in WIMS9 to produce homogenised cross sections for the whole core FETCH model was presented.

Spatial, energy, angle and scatter kernel convergence of the RZ and XY plane FETCH whole core models was investigated. Transport effects were found to be minimal (around 160 pcm) due to the amount of spatial homogenisation justifying the use of P1 diffusion theory. Quadratic basis functions on the coarsest mesh needed to define the material geometry were found to be sufficient for reducing the error associated with the Keff. Differences between using P0 and P1 scattering kernels was shown and the error in using the approximate transport cross section instead. Energy group structures decided suitable were 3, 6 and 11. This was based on a convergence analysis of the Keff and maximum power density. The effects of applying streaming corrections to the RZ and XYZ models was shown to reduce the Keff by around 1%.

Comparison of the WIMS9-FETCH model to the MONK9 model showed good agreement (less than 0.5% in most cases) for the Keff when not considering the reflector control rods. The control rod worth of the XYZ WIMS9-FETCH model showed around a 10% difference to the MONK9 result. Due to the minimal transport effects in the FETCH model this difference is considered due to the homogenisation models in WIMS9 but is recognised as the best currently achievable result.

Finally the variation of the FETCH models Keff with isothermal core temperature using different enrichments highlighted the issue of a too large excess reactivity in the model (and hence the design) for 14% enrichment. The 10% or 8% enrichment were shown to be more appropriate and will be investigated using coupled methods in the next chapter.
Synopsis

The coupled radiation transport thermal fluid dynamic 3D FETCH code is used to analyse a generic block type Very High Temperature Reactor. The FLUIDITY model produced as part of this research is described which includes the development of a submodelling method to capture the multiscale thermal physics processes inherent within the fuel assemblies. Coupled steady state results are used to analyse the generic reactor design for varying enrichments. Conclusions are finally stated as to the suitability of FETCH to model a generic block type VHTR.
6.1. Introduction

In this chapter the coupled radiation transport (RT) thermal fluid dynamic FETCH code is used to analyse the generic block type VHTR that was described in the preceding chapter. The preceding chapter analysed the design solely from an RT perspective for uncoupled eigenvalue steady state. The necessity to vary the design for limiting excess reactivity was proposed. The design option chosen was to vary the enrichment. The different enrichment designs will be investigated in this chapter using coupled methods.

The RT phase space resolution required to achieve a desired accuracy for these coupled simulations is inferred from the previous chapter analysis for uncoupled steady state results. Therefore simulations use P1 diffusion theory with streaming corrected anisotropic transport cross sections. The original spacial resolution for the RT is 408 quadratic elements in RZ and 21816 quadratic elements in XYZ. Due to computational constraints for the XYZ model 21816 linear elements are also used. The linear mesh must be recognised as retaining a larger spatial convergence error being inferred from the 1% error of the Keff.

A top plenum region was required for the FLUIDITY domain and is included in the RT model also as an increased graphite reflector region. The
top plenum increased the number of elements to 578 for RZ and 30906 in XYZ. The XYZ model uses the third hexagon material mapping, the whole hexagon material mapping model is not considered herein. The energy group structures used are the 3, 6 and 11 for the RZ model. For the XYZ model only 3 energy groups is considered as higher energy groups was considered too computationally expensive.

For all coupled simulations the variation in the helium coolant density and temperature variation is not considered in the feedback to the RT solver. The element wise material cross section mapping for the RT solver is interpolated from a predetermined database generated from WIMS9. Two types of database are used. Each has average temperature variation of the active fuelled region alone, other materials (such as the reflector and control rod) have no variation. The first database varies all the homogenised fuel region at the same temperature. The second varies the TRISO fuel kernel and all graphite components (fuel compact graphite and moderator block graphite) separately to produce a 2D grid to interpolate on. The difference in varying the temperature of the different graphite components in the 2D database is considered minimal so as to not need a 3D database. This assumes that the neutron importance of these regions (graphite in fuel compact and graphite in moderator) are similar due to the spatial scale of the unit cell geometry being less than the neutron mean free path in graphite.

This chapter is organised as follows. In the next section the VHTR FLUIDITY model used for coupled simulations is presented. This includes the description of the thermal submodel developed for capturing multiscale effects. The following section uses the coupled FETCH model to analyse the generic reactor design under steady state conditions for varying enrichments. Finally conclusions are stated with regard to the FETCH VHTR model and the generic VHTR design.

### 6.2. FLUIDITY VHTR Model

In this section the VHTR FLUIDITY model used for the coupled FETCH simulations is presented. The VHTR FLUIDITY model description includes the

- geometry and mesh,
• material properties and mapping,
• initial and boundary conditions,
• closure relations,
• dual thermal submodel formulation,
• and finally why FLUIDITY was used.

6.2.1. Geometry and Mesh

Coupling between the radiation transport and thermal fluid dynamic modules in FETCH involves exchanging volume element wise information. The element wise heat source is passed from the radiation to the fluids module. The fluids module passes an element wise material mapping (or attributes with which to interpolate a material mapping) back to the radiation module. This coupling relies on both modules reading in the same discretised mesh such that volume element number A in one is identical to volume element number A in the other. Therefore the mesh and material mapping deduced acceptable for the radiation module in the previous chapter is used for the fluids mesh also.

The FETCH mesh for both modules is added to by including a top plenum region above the top reflector of height 200cm (the actual height of the top plenum is unknown and the stated model height is estimated from literature design pictures of similar reactors). This is necessary for the FLUIDITY top boundary conditions being uniform and to allow FLUIDITY to calculate the mass flow rate through each reactor channel. The top plenum for the radiation module has the same material properties as the top reflector as opposed to a pure gas. Thus the number of elements is 578 for RZ and 30906 in XYZ.

6.2.2. Material Properties and Mapping

The two phase method within FLUIDITY is used to effectively model a homogenised porous media reactor geometry. The first phase is the helium gas phase and the second phase the solid. The solid phase has included within the momentum balance a very large absorption term such as to terminate all second phase movement. The gas phase uses the ideal gas law for an
equation of state with a background pressure of 70.7 bar. The porosity for the different materials is specified as input.

All the thermal fluid material properties are held constant within a simulation apart from the helium density that is calculated from equation of state. These are summarised in table 6.1. The viscosity of the helium is taken as $4.4 \times 10^{-4}$ g/cms. For the global homogenised solid phase model the material properties are taken as those of the graphite that forms the moderator and bulk of the fuel compact. This approximation is justified in that 3-4% of the solid within a fuel region is TRISO particles. The thermal fluid properties of the burnable poisons and control rods are not considered.

<table>
<thead>
<tr>
<th>Material</th>
<th>Density</th>
<th>Conductivity</th>
<th>Specific Heat Capacity</th>
</tr>
</thead>
<tbody>
<tr>
<td>U02</td>
<td>10.2</td>
<td>0.037</td>
<td>0.33</td>
</tr>
<tr>
<td>Buffer</td>
<td>1.0</td>
<td>0.005</td>
<td>1.725</td>
</tr>
<tr>
<td>PyC</td>
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<td>0.04</td>
<td>1.725</td>
</tr>
<tr>
<td>SiC</td>
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<td>0.16</td>
<td>1.725</td>
</tr>
<tr>
<td>Graphite</td>
<td>1.74</td>
<td>0.8</td>
<td>1.725</td>
</tr>
<tr>
<td>Helium</td>
<td>Ideal Gas</td>
<td>0.0037</td>
<td>5.195</td>
</tr>
</tbody>
</table>

Table 6.1.: Thermal fluid properties used for the FETCH VHTR model. Units are in Joules, grams, centimetres, seconds and Kelvin.

The delayed neutron precursors are represented by 6 groups Duderstadt and Hamilton (1976) with the properties given in table 6.2. The delayed spectrum is deduced from a fine 172 group sum to the condensed broad groups of the spectrum output from WIMS9. This implies that the same

<table>
<thead>
<tr>
<th>Delayed Group</th>
<th>Lambda</th>
<th>Beta</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.0124</td>
<td>2.2110E-4</td>
</tr>
<tr>
<td>2</td>
<td>0.0305</td>
<td>1.4673E-3</td>
</tr>
<tr>
<td>3</td>
<td>0.111</td>
<td>1.3132E-3</td>
</tr>
<tr>
<td>4</td>
<td>0.301</td>
<td>2.6465E-3</td>
</tr>
<tr>
<td>5</td>
<td>1.14</td>
<td>7.7050E-4</td>
</tr>
<tr>
<td>6</td>
<td>3.01</td>
<td>2.8140E-4</td>
</tr>
</tbody>
</table>

Table 6.2.: The six group delayed precursor data used for the FETCH VHTR model. Units are in inverse seconds for Lambda.
spectrum is used for each precursor. The delayed precursors are considered in the static eigenvalue calculations to form an effective spectrum that combines the prompt and delayed spectra with a delayed beta weighting. The energy released per fission is taken as 200MeV and is deposited instantly and locally. Gamma heating and decay heat are not considered.

6.2.3. Initial and Boundary Conditions

A fixed inlet gas velocity and density boundary condition is applied to the top plenum surface of the domain. The gas density inlet is calculated using the ideal gas equation of state at system pressure and at a temperature of 773 Kelvin. The velocity inlet is then calculated to give the correct inlet mass flow rate of 230Kg/s. The inlet gas phase temperature at the top of the domain is specified as 773 Kelvin. On the radial outer boundary of the cylindrical model (both RZ and XYZ) no normal flow boundary conditions are specified. In XYZ this involves using rotational boundary conditions. Zero diffusive temperature flux boundary conditions are used for both phases down the side of the cylinder domain and at the bottom. The bottom of the domain has a free outflow boundary condition for the gas phase that allows the advection of heat out of the domain.

The initial conditions consist of both phases having an isothermal temperature of 773 Kelvin, a uniform gas pressure of zero and a uniform gas velocity also of zero.

6.2.4. Closure Relations

The energy and momentum exchanges between the gas and solid phases is through the use of empirical correlations. For heat exchange the Dittus-Boelter Duderstadt and Hamilton (1976) correlation is used which is given by

\[ Nu = 0.023Pr^{0.33}Re^{0.8}, \]

(6.1)

where \( Nu \) is the Nusselt number that is related to the volumetric heat transfer coefficient, \( Pr \) is the fluid Prandtl number and \( Re \) the fluid Reynolds number. This correlation is standard for fluid flow through a cylinder channel. For momentum exchange the Blasius correlation Duderstadt and Hamilton-
ton (1976) is used which is given by

\[ f = 0.0791 Re^{-0.25}, \]  

(6.2)

where \( f \) is the fanning friction factor which is related to the volumetric momentum exchange coefficient. This correlation is also standard for fluid flow through a cylinder channel. These two correlations are used for all material regions of the domain through the use of a hydraulic diameter for non-circular channel regions. This includes the inner and outer reflector regions where the only gas flow present is that between the hexagonal blocks.

It is expected that most of the mass flow rate will be through the internal coolant and control channels. This flow in the porous model should only be able to move in the Z axis direction. A small (but unknown) flow rate will pass externally through the hexagonal block gaps. It is not possible to distinguish the two flows within the current FLUIDITY model. To restrict the dominant internal flow rate within coolant channels to be solely in the Z axis an anisotropic absorption term added to the R or XY directions would be needed. This is possible in FLUIDITY but was found to induce (or enhance) the occurrence of non-physical spurious chess board pressure modes. Therefore no anisotropic absorption term is added.

The gas phase is treated as a Newtonian fluid. Hence the stress term \( \tau \) in equation 2.27 for the gas phase is given by

\[ \tau^g_{ij} = 2\varepsilon^g \mu^g S^g_{ij} \]  

(6.3)

where \( \varepsilon^g \) is the volume fraction of the gas phase, \( \mu^g \) is the viscosity of the gas phase and the strain rate \( S^g_{ij} \) is given by

\[ S^g_{ij} = \frac{1}{2} \left( \frac{\partial v^g_i}{\partial x_j} + \frac{\partial v^g_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial v^g_k}{\partial x_k}. \]  

(6.4)

6.2.5. Dual Thermal Submodel Formulation

This section describes the formulation of a dual submodel to capture the double heterogeneity scales for energy exchange through the solid components of the VHTR fuel assembly. For a single heterogeneity (such as in an LWR fuel assembly) a single submodel alone would be required. For the
VHTR due to the double heterogeneity (fuel pins in hexagonal blocks and TRISO particles in fuel pins) either a double level submodel is required (a TRISO submodel within the fuel compact submodel, called a dual submodel) or a complicated domain submodel containing the TRISO structure within the fuel compact. The latter option is considered to be too complicated to construct and use within a whole core coupled model. Therefore the former is developed.

The dual submodel developed is a time dependent linear FEM based model used to solve the thermal energy equation over a domain that represents a repeated unit cell for that scale. This is similar to the way the homogenised group cross sections are generated in WIMS9. The domain of the submodel should accurately represent the heterogeneity that has been homogenised at this scale. To be precise this would be a full 3D whole fuel assembly model. However, having this as a submodel would defeat the purpose of originally homogenising materials which was to avoid excessive mesh and computer resources not possible yet. Therefore an approximation is taken, identical to the choice of unit cell for the WIMS9 calculations, in that the unit cell for the fuel compact submodel is the 2D equilateral triangle centred around one fuel compact as shown in figure 6.1. This approximation ignores any geometric Z axis variation within a fuel assembly. This is justified as the fuel compact extends 75cm (93.75%) of the 80cm height of the fuel assembly. A second approximation taken, again just as in the WIMS9 calculation, is to then change the geometry to concentric annuli such that the fuel compact submodel problem becomes 1D cylindrical.

To ease the linking between the global FETCH model and the fuel compact submodel the graphite moderator was not included within the submodel domain. Phase 2 of the global FETCH model then became solely this graphite moderator. This approximation assumes that there is no local temperature variation of interest in the graphite moderator between the fuel compact and the helium coolant channel wall. While the energy equation of phase 1 remains the same, the solid phase 2 energy equation is altered to

\[
\varepsilon_{p2} c_{p2} \rho_{p2} \frac{\partial T_{p2}}{\partial t} = \frac{\partial}{\partial x_{g1}} \left( \varepsilon_{p2} \kappa_{p2} \frac{\partial T_{p2}}{\partial x_{g1}} \right) + \alpha (T_{p1} - T_{p2}) + Q_{p2},
\]

where \( T_{p1} \) is the temperature of global phase 1 (helium coolant), \( T_{p2} \) the temperature of global phase 2 (graphite moderator), \( \varepsilon_{p2} \) is now the volume
fraction of graphite moderator within a global FETCH element (which will not be the same as the solid volume fraction used in the momentum equations for elements with submodels), $x_{g_i}$ is the global coordinate, $c_{p_{g2}}$ is the specific heat capacity of global phase 2, $\rho_{p2}$ is the density of global phase 2, $\kappa_{p2}$ is the thermal conductivity of global phase 2, $\alpha$ is the volumetric heat exchange coefficient between global phase 1 and 2 and $Q_{p2}$ is the energy source from the submodel to the global phase 2. The advection term is not included as it is not needed for the solid.

The fuel compact submodel is now given by a 1D cylindrical model of the fuel compact and surrounding gap. The energy equation for the submodel is given by

$$\varepsilon_{s} c_{p_s \rho_s} \left( \frac{\partial T_s}{\partial t} \right) = \frac{1}{r_s} \frac{\partial}{\partial r_s} \left( r_s \varepsilon_{s} \kappa_{s} \frac{\partial T_s}{\partial r_s} \right) + Q_s, \quad (6.6)$$

where $T_s$ is the submodel temperature, $r_s$ is the cylindrical radial dimension, $\varepsilon_s$ is the volume fraction of the materials within the submodel space (not the global space) that accounts for the use of a TRISO submodel (if there is no TRISO submodel then this is 1.0), $c_{p_s}$ is the specific heat capacity of the thermal submodel materials, $\rho_s$ is the density of the thermal submodel.
materials and $\kappa_s$ is the thermal conductivity of the thermal submodel materials. For the single submodel method $Q_s$ will be the fission source into the submodel domain (volume weighted correctly). If a TRISO submodel is used then $Q_s$ will be the source from the TRISO submodel to the fuel compact submodel.

The boundary condition on the fuel compact submodel is given by

$$T_s|_{r_s=\text{right}} = T_{p2}, \quad (6.7)$$

where the fixed Dirichlet temperature at the outer point of the domain, given by the time dependent global phase 2 temperature for the global element the submodel belongs to, will change with time. The gap is assumed to contain system pressure helium that has diffused through the graphite moderator pores and structural gaps. The fission heat source distribution across the fuel compact of the submodel is assumed to have a flat profile. The submodel is enforced for every global mesh element of the active core as temperatures are piece wise constant in FETCH. Within each time step (or FETCH iteration) the submodel is solved. The source into phase 2 from the submodel is given by

$$Q_{p2} = -A\kappa_s \left. \frac{\partial T_s}{\partial r_s} \right|_{r_s=\text{right}}, \quad (6.8)$$

where $A$ is conversion factor from a surface heat flux to a volumetric heat source that considers the relative volumes of the smeared geometry. For a negative gradient at the surface $Q_{p2}$ will be a positive source into the phase 2 element that contains this submodel. For a positive gradient this will become an absorption term.

The inclusion of a TRISO submodel proceeds identically to the fuel compact submodel but with a spherical coordinate domain. To ease linking between the TRISO submodel and fuel compact submodel the graphite in the fuel compact was not included within the TRISO submodel domain. The fuel compact in the submodel domain then became solely this graphite compact with an associated volume fraction $\varepsilon_s$. The TRISO submodel is now given by a 1D spherical model of the TRISO particle alone.

One TRISO submodel is used for every fuel compact submodel. The boundary conditions on the TRISO submodel are zero heat flux at the centre
(symmetric) and a Dirichlet temperature at the outer point given by the average temperature of the fuel compact of the submodel for which the TRISO submodel is linked to. The source into the fuel compact submodel from the TRISO submodel is given by the temperature profile at the outer edge of the TRISO submodel domain. This heat flux is volume weighted to account for the geometries involved. The fission heat source now becomes the source into the TRISO fuel kernel part of the TRISO submodel domain (gamma heating has been ignored as well as decay heat). The fission heat source distribution is assumed flat across the fuel kernel which is a good assumption as the flux across the TRISO is flat apart from at resonance energies.

Average temperatures of the fuel kernel and graphite fuel compact are calculated from the dual submodel for each global fuel assembly FETCH element. The graphite fuel compact and moderator (phase 2) temperatures are then averaged to give an average graphite temperature for each global FETCH element. This is used along with the average fuel kernel temperature to interpolate the element wise fuel assembly cross section set from a predetermined 2D grid. Cross section interpolation used in FETCH is linear so as to remain bounded and positive.

Averaging the graphite all together circumvents a 3D group constant grid between fuel kernel, graphite in fuel compact and graphite moderator (phase 2). A 3D grid would greatly increase the number of required WIMS9 calculations and complexity off all input files. For a 10 point temperature scale along each axis a 3D grid would require 1000 WIMS9 cycles. A 2D grid negates any difference in importance between the graphite in the fuel compact and the moderator with respect to temperature feedback (note that graphite has a mean free path of 2.5cm and the scale of the fuel compact submodel is 1.1cm).

The temperature of the TRISO coatings has not been taken into account for the graphite average temperature but are assumed the same temperature as all graphite in the WIMS9 calculations. The fuel assembly group constants are used to form a fission heat source density for a whole fuel assembly, as this is what the group constants represent. This is then weighted by dividing by the volume fraction of fuel kernel in a fuel assembly before being applied to the TRISO submodel. For a fuel compact submodel alone this weighting would be given by the volume fraction of the fuel compact in
the fuel assembly.

Thus the double heterogeneity of the fuel assembly is modelled with a
dual scale submodel coupled to the global solid phase 2 energy equation.
Fission energy is deposited promptly and alone into the TRISO fuel kernel submodel. Conduction transports this energy across the TRISO layers
which is then exchanged with the next scale being the surrounding graphite
in the fuel compact submodel. Conduction then transports energy across the
graphite fuel compact to the fuel moderator gap. Heat is then conducted
across the gap which is then exchanged with phase 2 of the global model.
Phase 2 (being the surrounding graphite moderator) then conducts the
energy globally around the core and exchanges energy with the coolant (phase
1). The coolant extracts the energy from the domain. Energy can also be
transferred in the opposite direction, from phase 1 to the TRISO submodel,
if needed.

Implicit time stepping is used for the dual submodel with the time step
determined by the global FETCH model (which may use adaptive time step-
ning for both thermal fluids and radiation transport). The non linear itera-
tions within FLUIDITY are used to ensure convergence between the global
and dual submodel scales. As each 1D fuel compact submodel and TRISO
submodel is assembled and solved individually and with the number of ele-
ments used being low, the matrix equations formed are solved directly and
individually by simple Gauss Elimination.

6.2.6. Why FLUIDITY is Used

The CMFD FLUIDITY model is used to represent the thermal fluid dynam-
ics of a VHTR for multiple reasons. Firstly as FLUIDITY is FEM based
it is capable of representing general geometries in 3D such as that used in
the VHTR model. Secondly FLUIDITY solves the general two fluid Navier
Stokes equations that includes compressibility and an ideal gas equation of
state. Thirdly as FLUIDITY is FEM based the coupling to a radiation
transport (or diffusion) FEM based model is theoretically and practically
simple using a one to one mapping of information element wise, provided
each component utilises the same mesh data. Fourthly FLUIDITY is a de-
veloped model that has been previously applied to a range of applications
including HTGR systems (pebble bed and fluidised bed Miles (2009)).
6.3. Steady State Analysis

In this section FETCH-B is used to analyse the generic VHTR design with varying enrichment using coupled eigenvalue and FLUIDITY calculations. As no steady state algorithm exists within FLUIDITY a time step marching approach to steady state is used. The coupled eigenvalue with FLUIDITY algorithm involves iterating between

- solving the eigenvalue problem,
- normalising the eigenvector to the design power of 600MW,
- forming an element wise power source for FLUIDITY,
- FLUIDITY then time steps a prescribed number of steps or duration,
- reforming an element wise material mapping for the radiation transport solver.

Coupled iterations continue until a total number is reached, the total FLUIDITY run time is reached or the coupled convergence tolerance of the Keff, flux and solid phase temperature is attained. Both the RZ and XYZ models are analysed for enrichments from 14% to 6%. The highest enrichment that gives a coupled Keff below 1.0 is then analysed using coupled control rod, eigenvalue and FLUIDITY calculations. This algorithm involves iterating between

- Coupled eigenvalue and FLUIDITY calculation,
- Control rod criticality search.

The control rod search is described in the Appendix B. These iterations continue until a total number is reached, the total FLUIDITY run time is reached or the convergence tolerance of the Keff and control rod tip height is attained. Note that the criticality search algorithm is designed for moving only one control rod or a collection in unison. Also the tolerances used for the coupled iterations including the control rod was set as $1.0E-06$. The tolerances used for the eigenvalue power iteration and matrix linear algebra solver were set as $1.0E-05$ for the XYZ models within the coupled iterations.

Initially simulations that do not use the thermal submodelling are performed. These are then followed by simulations that do use the thermal submodelling.
6.3.1. Without Thermal Submodel

In this subsection coupled steady state simulations are presented that did not use the thermal submodelling approach. Cross sections are tabulated for the fuel regions for the fixed temperatures 293K, 773K, 1273K, 1773K and 2273K. Linear interpolation is then used to generate an element wise material mapping for the neutronics.

The $K_{eff}$ obtained from the RZ model is presented in Table 6.3 using 3, 6 and 11 energy group structures. These simulations have the control rod fixed such as to have a tip height of 130cm, being the bottom height of the active core. The RZ model predicts that the highest enrichment possible

<table>
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<th>Groups</th>
<th>Enrichment (%)</th>
<th>Coupled $K_{eff}$</th>
</tr>
</thead>
<tbody>
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<td>3</td>
<td>14</td>
<td>1.12837</td>
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<tr>
<td></td>
<td>12</td>
<td>1.09689</td>
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Table 6.3: The $K_{eff}$ from coupled eigenvalue FLUIDITY simulations of the RZ model for different enrichments using 3, 6 or 11 energy groups. The control rods are fully inserted.

for initial critical full power from those investigated is 8%. The results also show that 3 energy groups is not sufficient using 8% enrichment to achieve a realistic steady state solution and thus requires 6% enrichment.

Results from simulations using the control rod criticality search for the RZ model in 3, 6 and 11 energy groups are presented in Table 6.4. Again no thermal submodelling was considered, the 3 group results used 6% enrichment and the 6 and 11 group results used 8% enrichment. The power
peaking factor is the ratio of the maximum power density to the average power density. The control rod tip height for the 3 group solution is higher than the 6 and 11 group solutions. This causes the neutron flux and hence power density to be concentrated in the axial regions below the control rod tip. As this is a small region of the active core the maximum power density is thus higher than the 6 and 11 groups. For the 6 and 11 groups the control rod tip is lower and the power density, shown in figures 6.2 and 6.3, is skewed towards the top half of the active core. This is due to the negative temperature reactivity coefficient with a downwards helium coolant flow.

The control rod tip height for the 11 group solution is slightly higher than the 6 group. This affects the power density distribution via increasing the value in the lower half of the active core causing a corresponding decrease in the upper half. This slight shift lowers the maximum power density, hence peaking factor, of the 11 group solution to the 6 group solution.

The maximum calculated steady state solid temperatures of the RZ models are all below 1300 °C. The gas and solid temperatures, gas velocity and pressure spatial distribution for the 11 group solution are shown in figures 6.4, 6.5, 6.6 and 6.7 respectively. A radial invariant pressure drop is calculated down the core due to drag. The gas velocity increases as it flows into the lower porosity regions of the top reflector region from the plenum. Gas velocity further increases by around a factor of two as the gas temperature increases in the active core region. This physical effect is captured due to the compressible formulation being solved. A significant volume of the lower

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Table 6.4: Results of RZ FETCH-B VHTR model from the coupled criticality search using 3, 6 and 11 energy groups. No thermal submodelling was considered, the 3 group results used 6% enrichment and the 6 and 11 group results used 8% enrichment.
ends of the inner and outer solid reflector is observed to be heated via conduction of energy from the core region. The temperature of these regions at steady state is a result of a balance of heat flux from the active core and heat removal from the coolant that flows between the hexagonal blocks. To maintain the inner and outer reflector at lower temperatures (such as to be an effective heat sink during a loss of cooling transient) the reactor design may benefit from the addition of coolant channels in the reflector regions adjacent to the active core. The gas temperature at the outlet from the coolant channel regions varies from about 1000 °C to 1288 °C.

The coupled $K_{eff}$'s obtained from the XYZ model using 3 energy groups for varying fuel enrichment is shown in table 6.5. Results are shown using linear and quadratic basis functions. No thermal submodelling was used. The 3 group linear basis functions results imply that the maximum enrichment possible of those investigated to achieve full power criticality with the control rods fully inserted is 10% for this model. Increasing the

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Table 6.5.: The $K_{eff}$ from coupled eigenvalue FLUIDITY simulations of the XYZ model for different enrichments using 3 energy groups. Results are shown for linear and quadratic basis functions used within the neutronics module BEANS. The control rods are held at fully inserted.

The number of groups was shown to decrease the calculated $K_{eff}$ for the coupled RZ model. This is in agreement with the previous chapter 5 where the 3 group isothermal XY and RZ models were shown to have just less than a 1% $K_{eff}$ difference to the 172 group calculations. This is used to extrapolate the conclusion that the coupled $K_{eff}$ from the XYZ model for quadratic
Figure 6.2: The RZ 6 group 8% enriched steady state power density (W/cc) calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. The colour scale is identical to that used for figure 6.3.
Figure 6.3: The RZ 11 group 8% enriched steady state power density (W/cc) calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. The colour scale is identical to that used for figure 6.2.
Figure 6.4: The RZ 11 group 8% enriched steady state gas temperature calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. The colour scale is identical to that used for figure 6.5. Units are in °C.
Figure 6.5: The RZ 11 group 8% enriched steady state solid temperature calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. The colour scale is identical to that used for figure 6.4. Units are in °C.
Figure 6.6: The RZ 11 group 8% enriched steady state gas velocity calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. Units are in cm/s.
Figure 6.7: The RZ 11 group 8% enriched steady state gas pressure calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. Units are in $g/cm.s^2$. The pressure shown is the overpressure, $\Delta P$, from the model reference pressure.
basis functions for the 12% enrichment case will be above 1.0 for converged energy groups. Hence for converged energy groups and spatial resolution the XYZ model predicts that the 10% enrichment case is the highest enrichment suitable to achieve full power criticality with control rods fully inserted. Note also that results from the previous chapter 5 showed that the WIMS9-FETCH XYZ model predicted a lower Keff for all control rods in compared to the MONK9 model by about 2%. Taking this into account the suggested enrichment is still closer to 10% than any other investigated.

Results from simulations using the control rod criticality search for the XYZ model in 3 energy groups are presented in table 6.6. No thermal submodelling was considered and linear basis functions were used for the neutronics. Quadratic basis functions were found to be too computationally prohibitive for this solution method using one processor, with expected simulation completion times estimated of the order of weeks. The coupled Keff

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<td>Control Rod Tip Height (cm)</td>
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</tr>
<tr>
<td>Max. Gas Temperature (°C)</td>
<td>1491</td>
</tr>
<tr>
<td>Max. Solid Temperature (°C)</td>
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</tbody>
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Table 6.6.: Results of XYZ FETCH-B VHTR model from the coupled criticality search using 3 energy groups. No thermal submodelling was considered, linear basis functions were used and the enrichment was 10%.

for this case is around 0.4% from the target of 1.0 as the control iterations had not fully converged, the simulation finished due to the FLUIDITY runtime (2.0E+06) being reached. Nevertheless the result is considered close enough to be analysed and it is recalled that this coarse mesh linear basis function resolution has a global 1% error compared to the more spatially converged quadratic equivalent. The maximum temperatures of the XYZ linear results are noticeably higher than the RZ results, although it is recalled that they used different enrichments. The power density and peaking factors are however reasonably similar between the XYZ and RZ results.
The temperature profiles at the bottom of the model (coolant outlet) of both phases are shown in figures 6.8 and 6.9. A noticeable rotational spiral effect is captured with the cooler green areas of the active channel regions corresponding to the positions of clusters of fuel assembly type 2's that contain a control channel hole. A large proportion of the inner reflector at the bottom is heated to around 1000 °C. Helium coolant outlet temperatures of from the active channel regions (coolant channels) varies by around 400 °C.

The axial variation of temperature for both phases is shown in figures 6.10 and 6.11 through an ZY plane slice at X equals zero. The maximum temperature of the coolant is at the model outlet at the bottom of the domain. The maximum solid phase temperature is at the bottom of the active fuel region. The inner reflector is not heated as much in comparison to the RZ model results shown in figure 6.4 which may be due to the simulation not reaching a fully converged steady state solution.

The axial variation of the gas phase velocity and pressure is shown in figures 6.12 and 6.13 respectively. The pressure decreases down the core due to drag and has larger values in comparison to the RZ model results shown in figure 6.7. The velocities can be seen to have mild oscillations in the XY direction within the fuel region. This non physical effect was not calculated for the RZ results and is considered to be caused by the FLUIDITY solver struggling to resolve the flow field from the plenum into the core and reflector regions. It is possible to prescribe anisotropic absorption coefficients within the FLUIDITY model to suppress XY direction flow in the fuel and reflector regions. However this caused the occurrence of non physical pressure checker board oscillations and was therefore not a viable option.

The power density is shown in figures 6.14 and 6.15. In the XY plane power density is generally peaked towards the central reflector. The reduction in power is seen in the third hexagons that have a control rod channel clustered in three's next to the central reflector. This reduced power results in the reduced temperature at the outlet for these regions as previously discussed. Axially the power density is peaked towards the lower end of the active core below the control rod tip height. These are the regions indicated by the yellow power density values. This is in contrast to the RZ results previously shown and is due to the higher position of the control rods within the XYZ model result.
Figure 6.8.: The bottom XY plane outlet of the helium coolant temperature from the 3 group XYZ FETCH-B model at steady state calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. Units are in °C and the colour scale is identical to that used in figure 6.9. Linear basis functions were used for the neutronics and no thermal submodelling was used.
Figure 6.9.: The bottom XY plane outlet of the solid phase temperature from the 3 group XYZ FETCH-B model at steady state calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. Units are in °C and the colour scale is identical to that used in figure 6.8. Linear basis functions were used for the neutronics and no thermal submodelling was used.
Figure 6.10.: The ZY planar cut at X equal zero of the helium coolant temperature from the 3 group XYZ FETCH-B model at steady state calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. Units are in °C and the colour scale is identical to that used in figure 6.11. Linear basis functions were used for the neutronics and no thermal submodelling was used.
Figure 6.11.: The ZY planar cut at X equal zero of the solid phase temperature from the 3 group XYZ FETCH-B model at steady state calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. Units are in °C and the colour scale is identical to that used in figure 6.10. Linear basis functions were used for the neutronics and no thermal submodelling was used.
Figure 6.12.: The ZY planar cut at X equal zero of the gas phase velocity from the 3 group XYZ FETCH-B model at steady state calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. Units are in $cm/s$. Linear basis functions were used for the neutronics and no thermal submodelling was used. The background colour is showing the porosity field so as to highlight the fuel, reflector and plenum regions.
Figure 6.13.: The outer cylinder view of the gas phase pressure from the 3 group XYZ FETCH-B model at steady state calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. Units are in $g/cm.s^2$. Linear basis functions were used for the neutronics and no thermal submodelling was used. The pressure shown is the overpressure, $\Delta P$, from the model reference pressure.
Figure 6.14.: The element wise power density of the 3 group XYZ FETCH-B model at steady state calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. The units of the power density are W/cc. Planar cuts leave one quarter of the core visible. Linear basis functions were used for the neutronics and no thermal submodelling was used.
Figure 6.15.: The ZY planar cut at X equal zero of the power density from the 3 group XYZ FETCH-B model at steady state calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. Units are in W/cc. Linear basis functions were used for the neutronics and no thermal submodelling was used.
6.3.2. With Thermal Submodel

In this subsection coupled steady state simulations are presented that did use the thermal submodelling approach. Cross sections are tabulated for the fuel regions for the fixed temperatures 293K, 773K, 1023K, 1273K, 1523K, 1773K, 2023K, and 2273K. A 2D cross section tabulation varying fuel kernel and graphite temperature separately was used. Bi-linear interpolation is then used to generate an element wise material mapping for the neutronics. Only simulations that search for the critical state are considered. For the RZ model only the 11 group case with 8% enrichment using quadratic basis functions for the neutronics was considered. For the XYZ model only the 3 group case with 10% enrichment using linear basis functions for the neutronics was considered.

The RZ results are shown in table 6.7 with and without using the dual thermal submodel. Inclusion of the dual submodel causes the calculated maximum power density and power peaking factor to decrease by around 9%. Temperatures of the two phases however only increase by about 1% with the inclusion of the dual submodel. The temperature difference from the maximum (average) fuel kernel temperature and the maximum solid phase (graphite moderator) temperature is 41 °C. The control rod tip height increases by around 1.5% with inclusion of the thermal submodel. The similar position of the control rod tip height resulted in a similar spatial distributions of the power density and temperatures with and without using the dual thermal submodel. These spatial distributions were presented in the previous section.

A characteristic temperature profile across the fuel compact and TRISO submodels is shown in figures 6.16 and 6.17 respectively. The temperature drop across the fuel compact submodel predominantly (90%) occurs across the gap between the fuel compact and what would be the surrounding graphite moderator. This gap was assumed to be occupied by system pressure helium and of a fixed thickness of 0.01cm. In reality the gap size will change due to thermal and radiative induced stresses acting on the fuel compact graphite and fuel assembly graphite moderator. The temperature drop across the TRISO submodel predominantly (80%) occurs across the buffer region. This buffer region consists of a reduced density porous graphite region.
Figure 6.16.: A characteristic temperature profile across the fuel compact submodel within the centre of the reactor domain for the RZ model using 11 groups.
Figure 6.17.: A characteristic temperature profile across the TRISO sub-model within the centre of the reactor domain for the RZ model using 11 groups.
Table 6.7.: The RZ 11 group FETCH-B steady state results of the coupled control rod, eigenvalue and FLUIDITY simulations with and without the dual thermal submodel (denoted ss). The maximum submodel temperature is the maximum of the average temperature of all fuel compact submodels. Similarly the maximum subsubmodel temperature is the maximum of the average temperature of all TRISO submodels. The solid temperature for the case with the dual submodel refers to the graphite moderator temperature.

The XYZ results are shown in table 6.8 with and without the dual submodel. Comparisons must consider that the case without the inclusion of the dual thermal submodel did not reach a fully converged critical steady state. Fine tuning of iteration parameters was necessary to provide a stable algorithm solution mainly because the FLUIDITY steady state had to be time stepped to. A balance had to be achieved between performing enough time steps such as to give stable coupling and computational simulation time. For the RZ model varying parameters was practical as simulation times rarely exceeded one hour. For the XYZ model however with simulation times of many days even for linear basis functions this was not rigorously possible, hence the non fully converged solution. The XYZ model with the dual submodel was more fortunate in iteration options chosen.

The maximum power density values are over 80% larger with inclusion of the dual submodel. The reason for this is that the control rod tip height is higher for the case with the thermal submodel. This increased tip height has resulted in spatial power density being further skewed to the bottom of the reactor. This is illustrated in figure 6.18 for the case with the dual
submodel in comparison to figure 6.15 for the case without. These results were obtained using linear basis functions for the neutronics. Previous results given in table 6.5 for no control rod search simulations show that if the more spatially converged quadratic basis functions were used the control rod tip height would be lower. This is because the coupled $K_{eff}$ for the 10% enrichment cases was higher and closer to 1.0 for quadratic compared to linear. This expected lower control rod tip height would reduce the power density peaking factor. The power density spatial distribution in an XY plane below the control rod tip height is shown in figure 6.19. With no absorber in the outer reflector the power density is quite uniform but decreased locally next to the inner reflector that contains burnable poisons. The green power density regions are the third hexagon parts of fuel assembly type 2 that contains a control channel hole.

The maximum temperatures of the gas phases are close between the cases of with and without the dual submodel, being different by 81 °C with a relative difference of around 5%. The maximum solid phase temperatures are closer but do not resemble the same materials (with the dual submodel the solid phase is the graphite moderator only). The dual submodel predicts a maximum average TRISO temperature higher than the generally accepted limit of 1600 °C. This limit is however for fault conditions not normal operation. The dual submodel gives a prediction of the TRISO kernel temperature higher than the average solid temperature. Due to the larger negative temperature reactivity feedback coefficient of the the TRISO kernel compared to the graphite, inclusion of the thermal submodel induces more negative feedback than considering average solid temperatures alone. Therefore to achieve criticality the control rod tip height would need to be higher for the case with the dual submodel.

6.4. Conclusions

In this chapter the coupled radiation transport thermal fluid dynamic FETCH-B model was developed and applied to the generic block type VHTR, which was previously described in the preceding chapter 5. The core mesh deduced acceptable from the previous chapter, that analysed the design neutronically alone, was used. This included and RZ and XYZ model that used linear or quadratic basis functions for the neutronics.
Figure 6.18.: The ZY planar cut at X equal zero of the power density from the 3 group XYZ FETCH-B model at steady state calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. Units are in W/cc. Linear basis functions were used for the neutronics and thermal submodelling was used.
Figure 6.19.: The element wise power density of the 3 group XYZ FETCH-B model at steady state calculated using the coupled control rod, eigenvalue and FLUIDITY algorithm. The units of the power density are W/cc. This is a XY planar cut at an axial position below the control rod tip height. Linear basis functions were used for the neutronics and thermal submodelling was used.
Table 6.8.: The XYZ 3 group FETCH-B steady state results of the coupled control rod, eigenvalue and FLUIDITY simulations with and without the dual thermal submodel (denoted ss). Linear basis functions were used for both simulations. The maximum submodel temperature is the maximum of the average temperature of all fuel compact submodels. Similarly the maximum subsubmodel temperature is the maximum of the average temperature of all TRISO submodels. The solid temperature for the case with the dual submodel refers to the graphite moderator temperature.

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The model geometry was modified for the coupled analysis to include a top plenum region for the fluid flow. The FLUIDITY model was described concerning material properties and phase exchange correlations used for heat and momentum balance. The development of a dual thermal submodel to capture the multiscale physics inherent within the homogenised model was described.

Steady state simulation results for both the RZ and XYZ models for varying enrichments was presented. These held the outer reflector control rods at fully inserted. For the RZ model these used the 3, 6 or 11 group structures given in the preceding chapter and for the XYZ model only the 3 group structure was considered. It was concluded that the highest enrichment possible with the capability to have a critical full power steady state was 6% for the 3 group RZ, 8% for the 6 and 11 group RZ and 10% for the 3 group XYZ. An argument was postulated to state that the XYZ model for converged (higher) energy group structure would still predict that the enrichment should be 10%.

The coupled control rod search, eigenvalue and FLUIDITY algorithm was
used to calculate the critical full power steady state for both the RZ and XYZ models. The RZ models maximum temperatures were all below 1300 °C. The XYZ model was run using linear basis functions for the neutronics as the quadratic was too computationally costly. The XYZ model maximum temperatures were higher than those of the RZ by over 200 °C. It is not known whether this is due to the different enrichments or an issue with the model. Noticeable XYZ domain effects were highlighted that the RZ model would not capture.

Steady state simulation results of critical full power using the dual thermal submodel were then presented. The RZ model used the 11 group structure and calculated the maximum mean TRISO temperature to be 1341 °C. Characteristic temperature profiles across the fuel compact and TRISO particle were shown. The largest temperature changes were shown to occur across the TRISO buffer region and the fuel compact to surrounding moderator gap. The XYZ model used 3 energy groups and calculated maximum mean TRISO temperatures for steady state higher than the accepted fault condition limit of 1600 °C. The control rod tip was sufficiently high for this simulation such that the spatial power density was severely peaked to the regions below the tip height. This resulted in a much larger maximum power density when including the dual thermal submodel in XYZ.

The necessity to fine tune iteration options associated with the coupled control rod, eigenvalue and FLUIDITY algorithm was discussed. Difficulty in achieving a steady state fully converged solution was due to having to time step in FLUIDITY to a steady state, which required balancing coupled stability and computational time. Fine tuning was possible for the RZ model but not rigorously an option for the XYZ. Use of the more spatially converged quadratic basis functions for the neutronics was considered too computationally prohibitive for use within these coupled criticality full power simulations, especially when repetition with fine tuning was required. Using quadratic basis functions for coupled eigenvalue and FLUIDITY (no control rod search) in the XYZ model took around 3-5 days to complete. The number of control rod iterations to achieve the target Keff was generally around 10. The expected number of days for the critical full power simulation in XYZ using quadratic basis functions is therefore around 30-50. Time profiling of the RZ 11 group case showed that over 90% of the time was spent in BEANS with the remaining spent in FLUIDITY. Note that time
profiling in general showed BEANS and EVENT to have a comparable computation speed. Use of the within code BEANS solver was generally 10-20% slower than EVENT whereas use of the PETSc solvers linked to BEANS was generally 20-30% faster than EVENT. This is stated to deduce that improved algorithms rather than actual coding methods would be required to reduce computational run time.

Therefore to have a usable XYZ model that is converged neutronically in space and energy would require an improved neutronic solution algorithm. Viable suggestions for this are:

- Use of coarse mesh rebalance acceleration Lewis and Miller (1993).
- Parallel solvers such as available in PETSc.
- Transverse leakage iteration similar to Nodal kinetics codes.
- Acceleration of higher order polynomial solutions (quadratic) by the lowest order linear, again similar to Nodal kinetics codes.
- Use of Nodal methods, analytic or expansion.

For the whole core geometric detail considered in this research the last suggestion to use a Nodal method is considered the most appropriate. A Nodal code, of which there are many ready available, would be better suited coupled to FLUIDITY than a conventional FEM code like BEANS or EVENT for this type of modelling. This would result in two model approximations needed compared to a FEM code. First the geometry would be restricted to hexagon prisms meaning that the circular outer reflector boundary would not be as well represented as in a FEM model. This error could be quantified through comparisons. Second the coupling mapping from the neutronics to FLUIDITY would be coarser. One nodal volume would represent the 6 finite elements that were used in FETCH-B. Again this difference could be quantified through comparisons of a simpler idealised problem. If it is considered important to capture the curvature of the geometry as in the FEM model then a hybrid model combining the Nodal method and FEM could be developed. This would use the Nodal method over the majority of the hexagonal domain and the FEM for the outer reflector regions that are non-hexagonal. Note that the use of a Nodal method over the FEM would not improve the model solution if both are converged but be computationally
more efficient. This is because they both solve the same equations. However in the VHTR case presented a converged FEM solution was not always possible in acceptable time (such as 1 week) where it is expected that a converged Nodal solution would be possible. Another benefit of using a Nodal code such as PANTHER is that they are standard Industrial tools so would be expected to have sufficient evidence of verification and validation and therefore be more usable directly than a academic research code.

One of the original intentions of this research was to analyse the generic VHTR for postulated transient faults such as control rod with drawl or ejection. This was not possible for four reasons being stated with decreasing importance as:

- Steady state analysis showed that the design required changes to be physically realistic.

- Steady state analysis showed that at normal operation maximum temperatures already exceeded accident limits.

- Steady state analysis showed that the solution method for the neutronics was too computationally prohibitive.

- The necessity for effectively a FETCH restart.

The first and second point suggest further research into the reactor design is required. The third point again suggests the use of a Nodal Kinetics code such as PANTHER that would also have the benefit of improved time stepping discretisations, being exponentially transformed. The fourth point is due to the necessity for realistic initial conditions for transient modelling. Control rod with drawl accidents are analysed from zero or full power. Analysing the generic VHTR from zero power would require the modelling of the start up control rods that are inserted into the fuel region. These were not considered in this research and their design details not known. The zero power condition is currently the only realistic initial condition possible in FETCH. A pseudo at power initial condition is possible through the initialisation of the time dependent neutronics with a normalised eigenvector solution. In this case though the FLUIDITY initial conditions would not match the neutronic initial conditions. Therefore a restart option for the FLUIDITY within FETCH is required so as to be able to initialise a tran-
sient from a coupled steady state solution. This however was not possible to achieve with the resources associated with this research.

The dual submodel presented in this chapter was heuristically derived. A more rigorous mathematical derivation is considered a necessity. Also the method could be improved via considering the sub scale temperatures as perturbations as was presented in Stainsby et al. (2008a) and Stainsby et al. (2008b) for similar reactors and intents. Qualifying the method through comparisons with numerical heterogeneous solutions of simplified problems that represent the same physics inherent within the VHTR is also needed.

Finally it is recognised that certain key physics are not represented in the current coupled model but could be included. These are:

- Radiative heat transfer between fuel assembly blocks.
- Temperature and fluence dependent FLUIDITY material properties.
- Xenon and Samarium poisoning.
- Burnup with fuel management.
- Improved fission energy deposition representation both spatially (gamma heating) and temporally (decay heat).
Chapter 7

CONCLUSIONS AND FUTURE RESEARCH

Synopsis

The primary purpose of this thesis is restated as to analyse the capabilities of the FEM based FETCH model to accurately model and make predictions of a generic block type VHTR, such as to be able to draw conclusions as to the suitability of the reactor design with regard to physical responses of interest. Initially a summary of each chapter is given followed by suggestions for future research.
7.1. Summary

In this section a summary of each chapter of this thesis is given.

- In the introductory chapter a summary of the historical evolution of nuclear energy was described. The future necessity for maintaining, or increasing, the global nuclear energy contribution was discussed. The international Generation IV initiative with the six selected designs was outlined. Following this a more detailed review of the Very High Temperature Reactor concept was given. This included advantages and disadvantages of the two variants, pebble bed and prismatic hexagonal block.

- In the second chapter the general theory involved in coupled radiation transport thermal fluid dynamic modelling of nuclear reactors was presented. Descriptions of mathematical methods used to model the individual components were briefly given. A review of methods applied to perform coupled modelling of nuclear reactor cores was then reviewed with a focus on V/HTR modelling. A more detailed derivation of the equations and methods inherent in the FETCH model used for this research was then described.

- The third chapter went into significant detail to describe the process and necessity of verification and validation (V&V). A definition of V&V was given followed by a review of processes involved in gathering evidence to support V&V assertions. An overview of previous V&V applicable to FETCH was given. The proposition that a continuously evolving code embodying the mathematical method requires a corresponding continuously evolving Quality Assurance process was taken. The framework adopted to perform continuous automated V&V was described. How this was applied to FETCH and the test cases that resulted from this was shown. The outcome of this process was one
reliable version of EVENT associated with FETCH. Another outcome was the production of a general multigroup diffusion FEM based code called BEANS that was used in the proceeding chapters. Enough verification tests were produced for EVENT and BEANS to assert that they are correctly implemented. A discussion of the verification procedures applied to the FLUIDITY version within FETCH was given. This was recognised to be in need of improvement, such as to be at a similar standard as that applied to EVENT and BEANS.

- The fourth chapter applied and developed a Sub Grid Scale (SGS) FEM based methodology to the multigroup neutron diffusion equations. The purpose of the method was to have the accuracy of a Discontinuous Galerkin (DG) formulation but with the computational efficiency of a Continuous Galerkin (CG) formulation. An initial review of the applicable methods was given. A detailed derivation of the SGS method analysed was then presented. Simplifications to the treatment of the outer domain boundary conditions were described followed by alternative methods to treat the diffusion term of the inner element. The method was analysed via direct application to four eigenvalue test cases. A difference in the methods behaviour between 1D slab geometry and 2D XY geometry was discovered. The method was also discovered to be unsuitable for problems with zero absorption coefficient (being a zero removal cross section neutronically) and unstable as this is approached. Methods to solve this were suggested and investigated but were are not considered rigorous alternatives. However, when the SGS formulation remained stable significant error reduction compared to CG was observed, for the use of linear Lagrange basis functions on all scales. The use of a higher order quadratic basis functions for the inner element solution had varied results.

- The fifth chapter analysed the generic block type VHTR solely with radiation transport models. Initially the WIMS9-FETCH model was partially validated via application to the IAEA HTR-10 initial criticality benchmark. Close agreement was found between the WIMS9 models and the known literature values. The necessity to model the streaming of neutrons in the outer reflector channels through the application of anisotropic diffusion coefficient corrections was shown. After
phase space convergence analysis the model was used to calculate the initial critical height to within 2.2% of the experiment. Further comparisons were made to other model results for varying core temperature and the control rod worth. Discrepancies were found and suggestions for them given. Following this initial benchmark the MONK9 model of the generic VHTR that was developed was described. This geometrically detailed model using continuous energy group cross sections was taken as a reference for the WIMS9-FETCH models. A range of increasing complexity models were compared between MONK9 and WIMS9-FETCH. The whole core FETCH models included an RZ and two different XYZ models. Phase space convergence analysis deduced an acceptable mesh, number of energy groups and that diffusion theory was suitable. When not considering the reflector control rods agreement between all the models (MONK9 and WIMS9-FETCH) was within 0.5% which was considered close. When including the reflector control rods larger differences were calculated with a 10% difference in the calculation of the control rod worth. Due to the minimal transport effects this was considered due to the control rod homogenisation (space and energy) methods used in WIMS9. Finally the chapter finished showing the variation of the whole core criticality factor with isothermal temperature increase. This highlighted that the generic VHTR design had too large an excess reactivity in cold state and lowering the enrichment to 10% or 8% was implied.

- The sixth chapter analysed the generic VHTR using the coupled methodology within FETCH-B. The required phase space resolution for the neutronics was inferred from the preceding chapter. The model constructed in FLUIDITY as part of FETCH-B was described. The development of a multiscale dual thermal submodelling method was then described. The purpose of this dual submodel is to capture the inherent multiscale physics that is effectively homogenised in the porous media FLUIDITY model. Steady state results for the RZ and XYZ model for varying enrichments were given. Different energy group structures were considered for the RZ model but only the 3 group structure for the XYZ model. These simulations resulted in the conclusion that the highest enrichment possible while being capable of full power critical-
ity was 10% for the XYZ model, 8% for the RZ model with 6 and 11 energy groups and 6% for the RZ 3 group model. Coupled control rod search, eigenvalue and FLUIDITY simulations then analysed the VHTR reactor using the RZ and XYZ models for with and without the use of the dual thermal submodel. Differences between the maximum predicted temperatures of the RZ and XYZ models was shown. RZ model maximum temperatures were just below 1300 °C, whereas the maximum XYZ model temperatures at steady state operation exceeded the accident limit of 1600 °C. The effect of the of the control rod height on the spatial power density was discussed. Finally conclusions stated that the reactor design required further change and the solution method used to solve the neutronics whole core balance would probably have been more computationally efficient if using a Nodal method.

7.2. Future Research

In this section future research directions are suggested.

In the third chapter conclusions it was stated that sufficient verification test cases were produced for EVENT and BEANS to assert that they are currently each correctly implemented as intended. However it is recognised that future verification of EVENT and BEANS (or other codes such as RADIANT) would benefit from the application of unit tests. These unit tests would check individual components of the code and be extremely fast. Also there is a necessity to be able to test the pre processor separately from the solver code. A version of FLUIDITY with an active continuous verification suite embedded within FETCH is strongly recommended. This is because currently there are no automated verification tests associated with the FLUIDITY in FETCH. This last point as well as the one concerning the pre processor are already under active research within the AMCG.

With regard to the SGS method applied to general diffusion equations further research into an alternative method that retains (or improves on) the positive qualities while not suffering from a singularity would be beneficial. This would not only be beneficial to the application of the method to neutron diffusion but also to any general context where an advection diffusion equation arises. If a stable method is possible then further investigation is
required on unstructured meshes and for time dependent problems. The use of different order and family of basis functions should also be investigated. Following this the method could be extended to be applied to the Even Parity transport equations or as a diffusion acceleration solver for a first order transport method. Also the SGS method developed as part of this research was directly compared only to the CG method. Future research should also include cross comparisons with various DG methods. This comparison should consider the accuracy, computational effort and actual ease of code manufacture and formula derivation.

The MONK9 code was capable of producing spatially detailed models to act as a reference solution for the deterministic codes. Improvement in the MONK9 model would come from the ability to have stochastically placed TRISO particles that are not clipped. Also all the comparisons shown in this research between MONK9 and WIMS9-FETCH only involved the criticality factor (a global result). Direct flux comparisons of regions defined separately from the model geometry would give an improved solution comparison that captures more local effects. This local region tally could correspond to the coarsest mesh of the FETCH model. With the desire to tally the flux solution more locally a larger number of samples would be needed than just calculating the core criticality factor. Thus a parallel version of the model would be useful. All of these points for future development of the MONK9 VHTR model are already part of the research plan (albeit for different applications) of the developing team at Serco Assurance and will be functional in future releases.

The radiation transport modelling of the control rods of the VHTR within WIMS9-FETCH showed a larger difference than any other component of the model in comparison to the MONK9 model. This is considered due to the homogenisation method used in WIMS9 to spatially smear and energy group collapse the cross sections. This difference may be reduced through the use of improved homogenisation methods such as Super Homogenisation (SPH). This would effectively iterate on the homogenised model such as to preserve reaction rates in regions plus one extra bonus. This extra degree of freedom resulting from being able to normalise the flux arbitrary could be the net current between the control rod region and the surrounding region. Further more the SPH method could be used to produce homogenised cross sections directly intended for diffusion models. The SPH method is an active
development within the WIMS code and may be available in future releases. However as control rod materials require no resonance self shielding the SPH method could be easily developed into the FEM based codes EVENT, BEANS and RADIANT.

To improve the computational efficiency of the whole core VHTR model in the geometric detail pursued in this research it is recommended that the FEM based neutronic solver be swapped for a Nodal Kinetics code such as PANTHER. This is expected to be substantially faster for both eigenvalue and time dependent problems. With a coupling of PANTHER to a version of FLUIDITY with active automated verification tests, design scoping studies of the VHTR can be pursued to optimise the design to be within material limits. Key physics that needs including within the model includes radiative heat transfer, improved material properties within FLUIDITY, Xenon and Samarium poisoning and a better representation of the spatial and temporal fission energy deposition. Analysis of the VHTR should also be considering fuel burnup and fuel management.

The geometric detail of the whole core model constructed would have been better represented in a Nodal Kinetics code. The FEM method is however capable of more complex 3D geometries. As more geometric detail is included in the whole core 3D model standard Nodal Kinetics codes are not applicable. Also diffusion theory becomes insufficient. A general FEM based radiation transport solver would then be needed. As the VHTR contains pure gas regions this would have to be a hybrid Even Parity to Ray Tracing model (such as historic EVENT) or a first order transport model (such as RADIANT). A more detailed FEM model could be constructed using a state of the art mesh generator that has more spatial detail of the control rods and channels in the VHTR. This would then alleviate the main difference observed between the MONK9 solution and the WIMS9-FETCH solution. The first order solver would require parallel solvers with an adaptive mesh such as to be rigorous and usable. Inclusion of this level of geometric detail is considered achievable. Further inclusion of geometric detail such as the fuel pins and further still to the TRISO particle level would require a massively parallel multiscale radiation transport solver. This is the general future aim of the RADIANT research within AMCG. Coupled to a massively parallel CFD solver such as FLUIDITY, a virtual reactor model is capable based on solving numerically the basic principle equation balances. This is the
general future aim of the FETCH research within the AMCG.
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The Behrens streaming correction formula is used to capture the physics of neutral particles moving through a material which has known holes. It applies a correction term to the diffusion coefficient for each hole present within the material. The formula given below is that used within the reactor physics code WIMS ANSWERS-WIMS and described by Newton (2010).

The Behrens corrected diffusion coefficient is given by

\[ D_{k,corr} = D_k - \sum_h \left( \frac{V_h}{V} \right)^2 \frac{t^h_k}{(e^{t^h_k} - 1)} D_k \sum_h \frac{V_h r_h Q_h}{v_k V}, \]  

(A.1)

where the following notation is used:

- \( k \) is the axial or radial direction,
- \( h \) is a hole index,
- \( D_{k,corr} \) is the corrected diffusion coefficient,
- \( D_k \) is the uncorrected diffusion coefficient,
- \( v_k \) is 2 for the axial direction and 4 for the radial direction,
- \( V_h \) is the hole volume,
- \( V \) is the smeared material volume (volume of all holes plus surrounding material),
• $r_h$ is the hydraulic radius,

• $Q_h$ is a hole shape factor (1.333 for infinite cylinder),

• $t_h^k$ is a direction and hole dependent factor defined below.

The direction and hole dependent factor $t_h^k$ is given by

$$t_h^k = \frac{2Vr_h}{3V_hD_k}. \tag{A.2}$$

If the hole is of rectangular cross section of side lengths $a_h$ and $b_h$ then the $Q_h$ factor is given by

$$Q_h = \frac{a_h + b_h}{2} \left[ \frac{1}{a_h} \ln \left( \frac{a_h + \sqrt{a_h^2 + b_h^2}}{b_h} \right) + \frac{1}{b_h} \ln \left( \frac{b_h + \sqrt{a_h^2 + b_h^2}}{a_h} \right) - \frac{(a_h^2 + b_h^2)^3 - (a_h^3 + b_h^3)}{3a_h^2b_h^2} \right]. \tag{A.3}$$
A control rod movement algorithm that is applicable for use in FEM based neutron kinetics solvers is described.

The regions of the FEM domain associated with the control rod channel are tagged using region identifications (ID). This effectively represents the control rod channel as a field across the domain with an ID value associated with the presence of control rod channel and another with its absence. The control rod channel is the space within which the control rod moves through. The control rod algorithm is restricted to the movement of the control rod solely in the z axis of the domain, hence is only applicable in 2D RZ and 3D XYZ geometries. The elements within each region associated with the control rod channel are analysed to determine their maximum and minimum z axis height via inspection of the local nodes associated with this element. This information is stored in dynamic arrays to be used to determine the control rod volume fraction distribution.

The mesh within the regions associated with control rod channels must be structured in the z axis. In 2D RZ geometry this restricts the mesh within these regions to Cartesian axis aligned quadrilaterals. In 3D XYZ geometry this implies that the top and bottom faces (with respect to the z axis) of the elements must be exact translations of each other in the z axis only. The XY cut plane of the mesh in these regions can be of any irregularity. Thus in 3D XYZ geometry the mesh within control rod channel regions can be formed from XY plane aligned triangular or quadrilateral zone stretched prisms, which form a type of wedge and hexahedral respectively.

These two restrictions (z axis movement and z axis structured mesh) are acceptable as nuclear reactors generally have z axis moving control rods and
are formed from geometric bodies that are typically aligned with the z axis.

Also, if the mesh within the control rod channel regions adapts then the
above information would need recalculating. However mesh adaptivity usu-
ally uses tetrahedral elements which are not suitable for the control rod
channel regions.

The region ID determine the spatial distribution of the control rod channel
within the model. A bank of control rods can be easily constructed through
the region ID being applied to spatially disconnected regions representing
the different control rod channels forming the bank. This will be effective if
the control rod channels are translations of each other in the XY plane. All
the control rods associated with the bank will then move in synchronisation.

Note that the control rod channel region need not extent to the edge of
the domain but could be totally (or partially) enclosed within the whole
domain.

An option is used to sp ecify whether the control rod is inserted from above
or below with respect to the z axis. Another option is used to specify the
initial z axis height of the control rod tip. It is the control rod tip height
that the algorithm moves. Knowing the initial control rod tip height and
whether the control rod is inserted from above or below the initial spatial
distribution of the control rod can be calculated. The control rod spatial
distribution can obviously only exist within the control rod channel regions.
A volume element wise control rod volume fraction field is formed where 1.0
represents rods fully inserted within the element and 0.0 represents control
rod fully withdrawn from the volume element. To calculate this volume
fraction field the maximum and minimum heights of each relevant volume
element are used to linear interpolate in the z axis if the rod tip is found
to reside within the middle of the element. This is why the restrictions on
the type of volume elements to form the control rod channel regions was
necessary.

The spatial distribution of the control rod channel and control rod volume
fraction are now used to form the element wise material properties of the
neutron kinetics solver. Note that the control rod is only influencing directly
the neutron transport model and not directly the thermal fluid dynamic
model. The material properties associated with the control rod are the total
and scattering cross sections. Fission cross sections are not considered. Each
control rod field has cross sections associated with the control rod channel
with and without the control rod in. The control rod channel element wise cross section is then formed by either

\[ \Sigma_{ele}^{CR} = \Sigma_{ele} + \alpha_{ele}^{CR} \Sigma_{CR}^{Rin} + (1 - \alpha_{ele}^{CR}) \Sigma_{CR}^{Rout}, \]  

(B.1)

or

\[ \Sigma_{ele}^{CR} = \alpha_{ele}^{CR} \Sigma_{CR}^{Rin} + (1 - \alpha_{ele}^{CR}) \Sigma_{CR}^{Rout}, \]  

(B.2)

where

- \( \Sigma_{ele} \) is the already determined volume element \( ele \) cross section,
- \( \Sigma_{ele}^{CR} \) the modified volume element cross section,
- \( \alpha_{ele}^{CR} \) the element wise volume fraction associated with control rod insertion,
- \( \Sigma_{CR}^{Rout} \) the cross section associated with the control rod channel without control rod in,
- and \( \Sigma_{CR}^{Rin} \) the cross section associated with the control rod channel with control rod in.

This flexibility allows the control rod cross sections to be added to already interpolated element wise cross sections (such as fuel regions interpolated in temperature) or to be the only cross section associated with regions. The former occurs where a control rod channel is part of a region associated with other homogenised materials whereas the latter occurs if the control rod cross section represents the exact detail required within the model.

In theory any number of control rods (or banks) can be modelled with no restriction on them spatially overlapping. This is useful in 2D RZ geometry when control rods are within the same annulus region but require separate treatment.

An algorithm was developed to move the control rod for both eigenvalue and time dependent problems. For time dependent problems each control rod had associated with it a maximum velocity, a maximum power fraction and a power level. Also for time dependent problems the option was included to have the control rod to either aim for a certain model power or to have movement initiated by a certain model power. The latter can thus be used
to model control rod safety systems (SCRAM) and control rod ejections (via setting the initiation power negative such that movement begins at the start of the simulation).

To aim for a power in time dependent problems at the end of each time step the power fraction between the model power and the control rod target power is calculated as

$$power\_fraction = \frac{Model\_power - control\_rod\_target\_power}{control\_rod\_target\_power}.$$  \hspace{1cm} (B.3)

Then if the $power\_fraction$ is greater than or equal to zero the velocity to move the control rod with is calculated as

$$control\_rod\_velocity = \left( \frac{\min(max\_power\_fraction, power\_fraction)}{\max_power\_fraction} \right)$$

$$\times \left| \max kontrol\_velocity \right|.$$  \hspace{1cm} (B.4)

else the velocity is found via

$$control\_rod\_velocity = \left( \frac{\max(-max\_power\_fraction, power\_fraction)}{\max_power\_fraction} \right)$$

$$\times \left| \max kontrol\_velocity \right|.$$  \hspace{1cm} (B.5)

Then if the control rod is inserted from above the sign of the control rod velocity is reversed such that the rod will move further into the domain if the power is too high. With the control rod velocity determined and a time step size known the new control rod tip height can be calculated for the end of the next time step. This control rod tip height is restricted to be within the maximum and minimum axial height associated with the corresponding control rod channel. With a new control rod tip height the control rod volume fraction is repopulated and the element cross sections reformed each time step as required.

Each separate control rod (or bank) for time dependent problems is moved independently of each other.

The control rod movement algorithm for eigenvalue problems is restricted to the movement of one control rod (or bank). The movement of more than one will not necessarily have a unique solution and would require a more complex algorithm. The control rod to be moved for an eigenvalue has the
following input options:

- An associated target Keff.
- An initial number of prescribed positions (minimum 2).
- Total number of control rod iterations.
- Control rod convergence tolerance.

The control rod eigenvalue algorithm works via iterating between prescribing a control rod tip height and solving the eigenvalue problem for that prescription. To determine the control rod tip height an initial database of tip heights and corresponding Keff’s is needed. The minimum number of entries in this database needed is 2, being the control rod fully in and fully out. The control rod tip height is then determined via:

- Searching the database for the closest from above and below Keff’s to the target Keff.
- If a Keff less/more than or equal to is not in the database the algorithm stops as the target Keff is not possible.
- Linear interpolation between the closest from above and below Keff’s to the target is used to determine an estimate of a new rod tip height.
- The new eigenvalue problem is then solved as normal and the Keff and tip height calculated added to the database.
- Iteration continues until a tolerance on the tip height is achieved or the maximum number of control rod iterations reached.

For each eigenvalue problem solved for a new control rod tip height the solution flux and Keff of the previous is used to initialise the current. Therefore as the control rod tip converges to achieve the desired Keff the number of eigenvalue solver iterations (inner and outer) will reduce improving the computational efficiency of the algorithm.

The above control rod algorithm was implemented as stated in the neutron kinetics code BEANS. The time dependent algorithm was also implemented in FETCH-E (EVENT-FLUIDITY) with the restriction that the control rod channel regions must be a part of the FLUIDITY domain. This is
because for this implementation the FLUIDITY generic fields were used to specify the spatial variation of the control rod. The eigenvalue algorithm is not implemented within the FETCH-E code but the initialisation of an EVENT eigenvalue run by FLUIDITY can be used with a control rod also defined (manual movement is therefore required to find a Keff). In each implementation the spatial distribution of the control rod and control rod channel for each set is output for visualisation. The time dependent variation of each control rod tip is output. Finally the control rod tip height and associated Keff database is output for an eigenvalue run from BEANS.
miniFLUIDS is a simple code embedded within the neutron kinetics codes EVENT and BEANS. It solves the within volume element heat equation with no advection or diffusion. It is used for simple coupled radiation transport thermal feedback which is useful for certain verification test cases. The miniFLUIDS thermal equation is given by

\[ c_p \rho \frac{dT}{dt} = S + \Gamma(T_0 - T), \]  

where

- \( c_p \) is the input heat capacity,
- \( \rho \) is the input density,
- \( T \) is the temperature to be calculated,
- \( T_0 \) is an input heat exchange temperature,
- \( \Gamma \) is an input heat exchange coefficient and
- \( S \) is the fission heat source.

The temperature equation is solved for each volume element where the time stepping uses a simple fully implicit scheme. The initial temperature is input also. The miniFLUIDS temperature can then be used to interpolate a new element wise cross section set. The miniFLUIDS within EVENT also solves for the delayed precursors with explicit coupling to the neutron flux equation.
This section provides evidence to quantify the error associated with applying the Behrens correction for anisotropic diffusion theory to capture streaming of neutrons in the control channels of the HTR-10 reactor benchmark problem. This evidence is used to evaluate the suitability of this method for the block type VHTR design.

It is usually common for the geometric design of a nuclear reactor to have an anisotropic nature. This anisotropy can arise due to the XY planar lattice fuel assembly arrays, such as those that occur in typical LWR and block type HTGR designs. Another geometrical anisotropy occurs because axial channels are included for the insertion of control rods. For a block type HTGR these control rod channels (which include channels for the emergency boron balls) are located within both the fuel assembly blocks and the outer reflector blocks. For a pebble bed HTGR these control rod channels are only located in the outer reflector blocks next to the core, which may be cylindrical or annular.

The control rod channels in the fuel assemblies of a block type HTGR and in the outer reflector blocks of a pebble bed HTGR in normal operation contain only partially inserted control rods. With the helium coolant...
filling these channels being effectively neutronically inert significant neutron streaming occurs within these channels. This streaming of neutrons induces a greater migration length in the axial direction thus increasing neutron leakage from the reactor system. An increase in neutron leakage will cause a decrease in core reactivity.

To accurately determine the whole core conditions of the neutron density field requires a model that accounts for the streaming effect in the control channels of the HTGR. For an explicitly represented channel a detailed transport model is required to capture the effect. This can be achieved through the use of Monte Carlo models such as MONK ANSWERS-MONK or first order deterministic models such as RADIANT Eaton (2004). Although these methods are of practical use for criticality alone calculations they are currently limited in use for multiphysics models such as FETCH applications. For coupled radiation transport thermal fluid dynamics modelling typically neutron diffusion theory is applied. Neutron diffusion theory is not capable of capturing the streaming in near void channels that are explicitly represented. Therefore these channels are homogenised with the surrounding material, being the fuel assembly block or reflector block. Alternatively the channels could be removed from the discretised domain and the neutron conservation within the channels represented by a ray tracing algorithm (such as in historic EVENT de Oliveira et al. (2001)) or via an analytic method that prescribes a boundary condition Williams and Cassell (2002) on the channel surfaces. These latter two models would however require a more detailed mesh to represent the channels and are of no use for an RZ geometry model. Therefore the channels are homogenised for the purpose of producing a coupled model within FETCH.

Homogenised (spatial and energy) cross sections are generated using the reactor physics model WIMS9 for all research associated with this thesis. Within WIMS9 there are four options to capture neutron streaming in holes through a geometry of interest. These are given by the option names ARIDNE, BENOIST, BONALUMI and BEHRENS. Each of these methods will produce corrected transport cross sections in the axial and radial direction. The BEHRENS method (described in Appendix A) is based on purely geometric factors. The other methods require the use of radial and axial collision probabilities. The BENOIST method Petrovic and Benoist (2002) is considered the most rigorous however the version available in WIMS 9 is only
applicable to a specific geometric case that is not relevant for the control channels in the outer reflector blocks of a HTGR. The BONALUMI option is only suitable for a tight lattice so is also not relevant here. The ARIADNE option is an approximation of the BENOIST option and is applicable to general geometries. An overview of the physics associated with calculating anisotropic diffusion coefficient (or anisotropic transport cross sections) is given in Williams (1974), Williams (1972) and Petrovic and Benoist (2002).

As the main aim of this thesis is the application of the multiphysics model WIMS9-FETCH to a generic VHTR that is still within the initial design phase, the simpler BEHRENS option (as opposed to the only other available option viable in WIMS9 being ARIADNE) is chosen to represent the streaming effects. The applicability of the BEHRENS option for capturing the streaming in a VHTR is inferred from an analysis on a simplified version of the HTR-10 criticality benchmark IAEA-TECDOC-1382 (2003). The original IAEA HTR-10 criticality benchmark is described in detail in section 5.2. A reference answer for the WIMS9-FETCH model is provided by a MONK9 model. So that a rigorous comparison is achieved the only difference between the two models (FETCH and MONK9) is that the FETCH model homogenises the streaming channels and the MONK9 model correctly represents them. All other geometries and materials are identical. To achieve this the MONK9 model embedded within WIMS9 is used so that the same two energy group cross sections (including the smeared pebble bed) are used with in the two models that are being compared. The comparison between the models considers the change in the criticality eigenvalue between with and without representing the channel streaming.

The simplifications to the HTR-10 criticality benchmark taken are:

- no account of neutron streaming in the pebble bed is considered,
- the graphite density of all reflector materials is taken as 1.74 g/cc,
- no boron impurities are considered in this reflector material,
- the pebble bed cone is approximated as a cylinder below the active core,
- all materials are at one temperature (15 °C),
- partial control rod insertion into the top reflector is not considered,
the helium inflow channels in the outer reflector are not considered,

- the control rod channels are all considered circular with a radius of 6.5 cm and extending axially from the height of the bottom of the cone to the top of the above plenum,

- all results in both models are for two energy groups with the thermal cut off being 4 eV (the thermal cut off in WIMS9).

The RZ geometry used within the FETCH models (both EVENT and BEANS) is shown in figure D.1. The more geometrically detailed MONK9 model is shown in figure D.2.

Initially a mesh refinement analysis on the FETCH models is used to find a suitable mesh that is converged for the eigenvalue to 10 pcm. Simulations are then performed for each model with and without a representation of the streaming. Both EVENT and BEANS models are used for the case without the streaming. The difference between the EVENT and BEANS simulations is that EVENT uses the P1 scatter data (the same as the MONK9 model) whereas the BEANS model uses the transport cross section produced by WIMS9. EVENT results for higher angular expansions are also performed. With regard to the application of the BEHRENS streaming correction this is only applicable for use with BEANS, not EVENT. This is because BEANS is an anisotropic diffusion coefficient model whereas EVENT is an isotropic material Even Parity transport model. Comparison between the models is via the eigenvalue which will provide a measure of the global net change in leakage when including the streaming. Results are shown in table D.1.

The difference in the Keff of the EVENT P1 and EVENT P9 simulations is about 430 pcm. This shows that there are still some appreciable transport effects not captured by a diffusion model when using these two group cross sections.

A noticeable difference exists between the EVENT P1 result and the BEANS no BEHRENS result, with the difference in Keff being 1621 pcm. The only difference between these two models is the treatment of the anisotropic scatter terms, with EVENT correctly using the P1 data whereas BEANS uses the transport cross section.

The change in Keff for the MONK9 model when including the streaming channels explicitly is 1390 pcm. The corresponding change in the Keff for
Figure D.1.: The geometry used within the FETCH models of the simplified HTR-10 problem. In this model the streaming channels are homogenised into the surrounding graphite reflector annulus. Thus the whole geometry can be represented in RZ coordinates where the left hand axis is the central Z axis. The dark blue material is the core, the light blue material the approximate cone region, the grey material the upper plenum, the red material the homogenised streaming channel region and the remaining material the generic reflector graphite.
Figure D.2: The geometry used within the MONK9 model of the simplified HTR-10 problem. In this model the streaming channels are explicitly represented. The yellow material is the core, the green materials are the upper plenum and streaming channels and the purple material is the reflector regions.
Table D.1.: Eigenvalue results for the simplified HTR-10 problem for comparison of the different models abilities to capture channel streaming.

<table>
<thead>
<tr>
<th>Model</th>
<th>Keff Eigenvalue</th>
</tr>
</thead>
<tbody>
<tr>
<td>MONK9 no channel</td>
<td>1.1757 (stdv 0.0002)</td>
</tr>
<tr>
<td>MONK9 with channel</td>
<td>1.1618 (stdv 0.0004)</td>
</tr>
<tr>
<td>EVENT P1</td>
<td>1.16971</td>
</tr>
<tr>
<td>EVENT P3</td>
<td>1.17304</td>
</tr>
<tr>
<td>EVENT P5</td>
<td>1.17384</td>
</tr>
<tr>
<td>EVENT P7</td>
<td>1.17396</td>
</tr>
<tr>
<td>EVENT P9</td>
<td>1.17401</td>
</tr>
<tr>
<td>BEANS no BEHRENS</td>
<td>1.15350</td>
</tr>
<tr>
<td>BEANS with BEHRENS</td>
<td>1.13656</td>
</tr>
</tbody>
</table>

the BEANS model when including streaming via BEHRENS is 1694pcm. Therefore there is about a 20% difference between the MONK9 and WIMS9-FETCH models with regard to capturing the streaming effect. This result is considered satisfactory considering that the difference between the EVENT P1 and BEANS no BEHRENS Keff’s is 1621pcm, which is comparable to the BEHRENS streaming correction and greater than the MONK9 streaming effect. Transport cross sections (hence diffusion coefficients) are required to apply the streaming corrections which in itself induce a larger error than not applying any streaming corrections for this problem definition.

In conclusion, when extrapolating the HTR-10 simplified model results to the VHTR design it is considered satisfactory to use the simplest option available within WIMS9 (BEHRENS) to capture the channel streaming effects. Future research could consider the ARIADNE option within WIMS9 to reduce the 20% difference to the MONK9 reference. However, this must be considered with a knowledge of the error induced from using the transport cross section rather than the actual P1 scatter data correctly. For the simplified HTR-10 model analysis this error was shown to of a comparable size to the actual streaming effect. An adaptive in angle first order deterministic method Buchan et al. (2008) or hybrid Even Parity with ray tracing method de Oliveira et al. (2001) would both be suitable numerical models capable of representing the streaming channels using the mesh shown in figure 5.7. For these models to be of a practical use for transient multiphysics
analysis (within a FETCH context) parallel computation is a necessity. This is considered the main direction for future numerical research for radiation transport analysis of HTGR’s within a multiphysics framework. Finally the comparison for the deterministic WIMS9-FETCH model relied on taking the MONK9 model as a reference. Therefore MONK9 itself should be directly validated for the HTR-10 criticality benchmark for completeness.