Development of a Long-Life Core
for Commercial Marine Propulsion

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Glossary

$ (dollar unit) Refers to the reactivity margin between delayed and prompt critical.

**ABWR** Advanced Boiling Water Reactor.

**AGR** Advanced Gas-cooled Reactor.

**AO** Axial Offset - defined as the difference in power between the top half of the core and the bottom half of the core, divided by the total core power.

**AOA** Axial Offset Anomaly - defined as a significant (>3%) deviation of the axial offset in the operating core from its predicted value.

**BOL** Beginning of Life, i.e. $t = 0$.

**BP** Burnable Poison.

**BPP** Burnable Poison Pin - a fuel rod containing burnable poison.

**BWR** Boiling Water Reactor.

**CANDU** CANada Deuterium Uranium, a type of pressurised heavy water reactor.

**cermet** Ceramic-metallic fuel such as $\text{UO}_2$ particles in a zirconium alloy matrix.

**CF** Capacity Factor - defined here as the average power output over the system’s life divided by its maximum power output.

**CRB** Control Rod Blade.

**CRDM** Control Rod Drive Mechanism.

**CVCS** Chemical Volume and Control System.

**CZP** Cold Zero Power - the core state once shutdown has occurred and sufficient time has passed that the coolant temperature is at room temperature (taken to be $20^\circ$C).

**DBA** Design Basis Accident.

**DCF** Dual Cooled Fuel.

**DDC** Distributed Doppler Coefficient.

**Denaturing** Dilution of one isotope relative to another, for instance reducing the concentration of $^{235}\text{U}$ by the addition of $^{238}\text{U}$.

**EOL** End of Life.

**FG** Fission Gas.
FGR Fission Gas Release.
GHG Greenhouse Gas.
GW.d/tHM Gigawatt days per tonne of heavy metal - a unit of burnup.
HBS High Burnup Structure.
Heavy Metal All elements with an atomic number greater than actinium’s atomic number which is 89.
HEU High Enriched Uranium - defined as having a $^{235}U$ concentration greater than 20 wt.%.
HFP Hot Full Power - the core operating state when it is operating at 100% power.
HM Heavy Metal.
HP High Poison - an axial region of the core containing a high concentration of burnable poison.
HPP Hot Partial Power - the core state when it is operating at 25% of its maximum power.
HZP Hot Zero Power - the core state immediately after shutdown has occurred from full power operation and the coolant temperature across the core is equal to the inlet temperature.
LEU Low Enriched Uranium - defined as having a $^{235}U$ concentration less than 20 wt.%.
LOCA Loss of Coolant Accident.
LP Low Poison - an axial region of the core containing a low concentration of burnable poison.
LWR Light Water Reactor.
MOX Mixed Oxide fuel which is a mixture of plutonium and uranium oxide.
MTC Moderator Temperature Coefficient.
PCI Pellet Clad Interaction.
PHWR Pressurised Heavy Water Reactor.
PT Pressure Tube - the component of a CANDU reactor that contains the fuel rods.
PWR Pressurised Water Reactor.
RCCA Rod Control Cluster Assembly.
RCP Reactor Coolant Pump.
RPF Relative Power Fraction is the relative power of one core unit (for example an assembly) relative to the average power of all core units.
RPV Reactor Pressure Vessel.
SB Soluble Boron.
SBF Soluble Boron Free.
SG Steam Generator.
**SGTR** Steam Generator Tube Rupture.

**SLC** Standby Liquid Control - a system employed in some BWRs that ensures shutdown from any reactor state via the injection of soluble boron.

**SMR** Small Modular Reactor.

**SNF** Spent Nuclear Fuel.

**SS** Stainless Steel.

**Ternary Fission** A nuclear fission process whereby three nuclei are produced instead of the usual two.

**WZP** Warm Zero Power - the core state once shutdown has occurred and the coolant temperature has reached 100°C.
Abstract
The University of Manchester
Aiden W Peakman
Doctor of Philosophy in the Faculty of Engineering and Physical Sciences
Development of a Long-Life Core for Commercial Marine Propulsion
23/09/2014

If international agreements regarding the need to significantly reduce greenhouse
gas emissions are to be met then there is a high probability that the shipping industry
will have to reduce its greenhouse gas emissions. For emission reductions from ships
greater than around 40% then alternatives to fossil fuels - such as nuclear energy - will
very likely be required.

Whilst nuclear powered ships have successfully operated at sea for a number of
decades, these have been primarily naval systems (or derivatives of naval systems such
as icebreakers) and a few demonstration projects using reactors with low power outputs.
The operational requirement for large civilian vessels (for example high capacity factors
and limited personnel) mean the naval and past demonstration reactor systems are ill-
suited for use in the current fleet of commercial container ships.

There have been relatively few studies performed addressing the likely requirements
upon core design a marine reactor would have to meet. This study addresses those is-
sues and also implements a Pressurised Water Reactor core design capable of achieving
these requirements. Furthermore, in order to simplify reactor operation for a limited
number of personnel on board, the chemical reactivity control system has been elimi-
nated during power operation. This has resulted in a novel low power density core that
does not require refuelling for 15 years. The neutronic and fuel performance behaviour
of this system has been studied with conventional UO$_2$ fuel and thorium-uranium oxide
((Th,U)O$_2$) fuel.

With respect to (Th,U)O$_2$ fuel there has been limited analysis comparing the perfor-
mance of key fuel characteristics, such as fission gas release and thermal conductivity,
as a function of uranium content in (Th,U)O$_2$ fuel and their impact on fuel behaviour.
Furthermore, the performance of neutronic codes for modelling $^{232}$Th and $^{233}$U from a
variety of experiments using modern nuclear data libraries (post 1990) is lacking. Both
of these issues are addressed in this study.

Whilst it is frequently stated that thorium-based oxide fuel is superior to UO$_2$ fuel
it was found that due to the sensitivity of thermal conductivity on temperature and
uranium content this was not true for the core designed in this study. The (Th,U)O$_2$
core showed no net economic benefits with respect to the UO$_2$ core and it was found
that the fuel performance of (Th,U)O$_2$ fuel was worse than the UO$_2$ fuel in the reactor
designed here. The UO$_2$ core design, however, was able to satisfactorily meet the
majority of requirements placed upon the system.
Declaration

The only portion of the work referred to in this thesis that has been submitted in support of an application for another degree or qualification of this or any other university or other institute of learning was part of the Monte Carlo benchmarking work relating to Uranyl Nitrate Solution Experiments.
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Finally I am very thankful for the help I have received from Charlotte Moon.
Chapter 1

Introduction

1.1 Shipping Emissions

The primary reason for investigating alternative power sources for shipping is to substantially reduce the shipping industry’s contribution to anthropogenic climate change. The global shipping industry emits around 1.1 giga tonnes (Gt) of CO$_2$eq greenhouse gases (GHG) per year, where the unit CO$_2$eq is used to quantify the warming impact of different GHGs relative to CO$_2$ [1]. Furthermore, most ships utilise so-called heavy fuel oils which are blends of the residues and distillates that are derived from various petroleum refinery processes [40]. The benefit of this fuel type is its low cost in comparison to other petroleum forms [41]. However, the sulphur content of heavy fuel oils is very high (> 1%) in comparison to the Ultra-Low-Sulphur Diesel used in land based vehicles in most countries (< 0.005%) [41, 42]. Sulphur and the nitrogen compounds present in all diesel fuels are oxidised when undergoing combustion resulting in sulphur oxide (SOx) and nitrogen oxide (NOx) pollutants. Hence another reason for investigating alternative power sources for ships is environmental legislation requiring reductions in SOx and NOx emissions. However, in the case of SOx and NOx emissions, these can be readily reduced, at some cost, by the refinement of the marine fuel and the addition of systems that process exhaust wastes [42, 43, 44].

The emission of around 1.1 GtCO$_2$eq per year from the shipping industry is a relatively small proportion (around 2%) of the total anthropogenic GHGs emitted, which were approximately 50 GtCO$_2$eq in 2010 [24]. However, most nations have agreed that the global mean surface temperature, relative
to those before industrialisation, should not be allowed to rise above 2°C [45]. In order to ensure that the probability of going above this level is low, drastic reductions in global GHGs are required.

Figure 1.1: Greenhouse gas (GHG) emission scenarios along with corresponding GHG concentration by the year 2100. A concentration of 450 ppm CO$_2$eq and a concentration of 650 ppm CO$_2$eq result in predicted temperature rises by the year 2100 of around 1.6 and 2.6°C respectively [24].

To limit the extent of future global warming the concentration of greenhouse gases must be limited and therefore what is of interest is the cumulative emissions of GHGs over a particular time period. It is predicted that emitting around 1800 GtCO$_2$eq over the time period from 2012-2100 would likely result in the concentration of GHGs by the year 2100 of around 450 ppm with a corresponding temperature rise of around 1.6°C [24]. For comparison, cumulative emissions over the same period of
around 2700 GtCO$_2$eq would be likely to result in a temperature rise of around 2.6°C$^1$ [24].

Figure 1.1 shows how different cumulative emissions result in different predicted temperature rises by the year 2100. The emission scenarios show that having the emission rate peak earlier (for instance in the year 2020) results in considerable differences in sustained emission reduction rates to ensure GHG concentrations are ≤ 650 ppm. In constructing Figure 1.1 it has been assumed that from the year 2012, up until the time at which the peak emission rate occurs, emissions increase by 2.2% per year, which was the average yearly increase from the year 2000 to 2010 [24]. In addition, negative emission scenarios (whereby GHGs are removed from the atmosphere at a higher rate than they are being released into the atmosphere) are considered unfavourable due to the considerable thermodynamic cost associated with such strategies [6].

Figure 1.1 shows that for GHG concentrations to be ≤ 650 ppm then emission rates by 2100 must be ≤ 10 GtCO$_2$eq per year. Hence as shipping currently accounts for emissions of 1.1 GtCO$_2$eq per year then as long as other sectors of the economy are able to reduce their combined emission ≤ 9 GtCO$_2$eq per year then the limit of around 10 GtCO$_2$eq per year would not be surpassed. However, whilst for many economic sectors technology exists to reduce emissions by around 90% [24], this is not the case for at least the four sectors outlined in Table 1.1.

The current total emissions from the sectors outlined in Table 1.1 are around 10.7 GtCO$_2$eq and have the potential to reduce emissions to around 7.6 GtCO$_2$eq without the need to radically depart from current technology/fuel sources. Complicating matters is that demand from these four sectors is expected to approximately double by around 2050 [1, 46, 2, 3]. This implies that that even if these four sectors were to implement the reductions shown in Table 1.1, their combined emissions would still be around 15 GtCO$_2$eq, which is beyond the permissible limit of around 10 GtCO$_2$eq per year. Therefore, either GHGs are removed from the atmosphere to compensate for the emissions from the sectors in Table 1.1, or efforts are made to further reduce emissions from these sectors. It is therefore necessary to attempt to find ways to reduce emissions for the sectors outlined in Table 1.1 and in this study the focus is on the shipping sector.

$^1$It is important to note that predicted temperature rise by the year 2100 does not constitute the equilibrium temperature rise as even if emissions were to stop being emitted at this date, positive feedback mechanisms may be in place that cause the temperature to rise further before reaching an equilibrium value. For instance, at higher temperatures it is expected that greater quantities of polar ice melt occur and hence alter the reflection (albedo) coefficient over a time period beyond that over which GHG emissions have been emitted.
Table 1.1: Economic sectors that were identified as currently not being amenable to large emission reductions, along with potential emission rates assuming current technological options are deployed to reduces emissions [1, 2, 3, 4, 5]. Appendix A.1 briefly outlines the assumptions in constructing this table.

<table>
<thead>
<tr>
<th>Sector</th>
<th>Current Emission Rates</th>
<th>Achievable Emission Rates</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air transport</td>
<td>0.75 GtCO₂eq/y</td>
<td>0.75 GtCO₂eq/y</td>
</tr>
<tr>
<td>Industrial process emissions</td>
<td>3.5 GtCO₂eq/y</td>
<td>3.5 GtCO₂eq/y</td>
</tr>
<tr>
<td>Shipping</td>
<td>1.1 GtCO₂eq/y</td>
<td>0.66 GtCO₂eq/y</td>
</tr>
<tr>
<td>Agriculture</td>
<td>5.3 GtCO₂eq/y</td>
<td>2.7 GtCO₂eq/y</td>
</tr>
</tbody>
</table>

Figure 1.2: Current emissions by the world shipping fleet in GtCO₂eq by ship type [25]. Note that the tankers have been subdivided into crude oil tankers and product tankers as they are distinct from one another (crude tankers are around a factor of ten larger). Furthermore, both of these tanker types are distinct from bulk carriers that transport large quantities of items such as coal or grain, which typically have storage capacities somewhere between product and crude oil tankers.

Figure 1.2 displays a breakdown of current emissions from shipping by ship type with emissions from container ships dominating (emitting around 0.3 GtCO₂eq).

Given that container ships’ historic emission growths are strongly correlated with global economic growth (which is unsurprising given their function in world trade) their future emission rates are expected to considerably increase [1]. Without the adoption of a range of technologies to improve efficiency (which are discussed below) emissions could increase by around 0.7 to 1.0 GtCO₂eq on top of current emissions of around 1.1 GtCO₂eq, assuming annualised growth of between 2 and 3% in global Gross Domestic Product (GDP). Unless surges in demand arise from the other sectors outlined in Figure 1.2, then container ships would still likely dominate emissions from ships. A similar conclusion was drawn in Ref. [25].
### 1.2 Alternative Fuels

<table>
<thead>
<tr>
<th>Fuel Type</th>
<th>GHG Intensity (gCO\textsubscript{2}/kWh(e))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coal</td>
<td>800</td>
</tr>
<tr>
<td>Heavy Fuel Oil</td>
<td>500</td>
</tr>
<tr>
<td>Natural Gas</td>
<td>400</td>
</tr>
<tr>
<td>Biofuels</td>
<td>200</td>
</tr>
<tr>
<td>Solar PV</td>
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</tr>
<tr>
<td>Wind</td>
<td>12</td>
</tr>
<tr>
<td>Nuclear</td>
<td>12</td>
</tr>
</tbody>
</table>

Table 1.2: Greenhouse gas (GHG) intensity per kWh of electricity by fuel type [6, 7].

Table 1.2 shows the emission intensity of various fuel types that have been used in the past (coal), present (heavy fuel oil) and which could be used in the future. Natural gas is likely to only constitute a minor improvement in emission reduction relative to the other fossil fuels.

From the outset it is assumed in this work that returning to ships powered entirely powered by sail, as was the case prior to the 18th century, would be unfavourable [43]. Current ships, in particular those that carry large quantities of cargo, are simply too large to be powered entirely by wind. In fact for these large ships it is unlikely that propulsion augmentation systems (sails and kites) would contribute to more than a 3% reduction in emissions from these ships [25]. It would require an extreme departure from current ship designs that have over centuries steadily become larger in order to benefit from the economies of scale associated with carrying ever more cargo on a single ship and realising large gains in efficiency. By adopting smaller slower ships it would be expected that significant increases in costs associated with transporting goods by ships would arise [47].

The shipping sector as a whole may be able to achieve around 30% reductions in GHG emissions via ‘mission refinement’ (travelling at slower speeds) and resistance reductions between a ship’s hull and the seawater [25]. Ref. [25] concludes that further optimisation of engines and propellers are unlikely to give gains of more than around 5%. Hence, whilst considerable reductions of perhaps up to 40% in CO\textsubscript{2} emissions may be possible, if total GHG emissions from the shipping sector were to double then the adoption of this suite of technologies would not offset the predicted increase in GHG emissions. Therefore alternative fuels must be considered to further decrease ship emissions.
Besides wind (which would only give a small reduction in emissions of around 3%) the utilisation of photovoltaic (PV) cells is another potential option. However, the use of PV cells on large ships appears unlikely to constitute reductions of more than the estimate for wind [25].

1.2.1 Biofuels

Biofuels are a fuel source which may contribute to emission reductions on a much larger scale than is achievable with wind or solar for powering large shipping vessels. However, their CO₂ intensity is likely around 200 gCO₂ per kWh(e) which is significantly higher than other low-carbon energy sources, such as wind, PV and nuclear, whose emissions are all below approximately 50 gCO₂/kWh(e) [7]. Therefore this limits the extent of reduction relative to the use of fossil fuels, which all have emission intensities of greater than 400 gCO₂/kWh(e) [7].

![Figure 1.3: Power densities for various biofuels, taken from [6]. "In the case of tropical plantations it has been assumed [6] genetic modification, fertiliser application and irrigation result in power densities approaching around 2 W/m²."

Another issue with regards to biofuels, as shown in Figure 1.3, is their very low energy density of around 0.5 W/m² and therefore large land requirements to grow the crops, which will likely result in reducing the amount of available land for food production.

Figure 1.3 shows that some plants have significantly higher power density than others. However this often requires the plants to be grown in tropical locations which raises the concern that rain forests

\footnote{Whilst some crops (such as jatropha) are able to grow on land that is unsuitable for food production, utilising this land comes at the significant penalty of lower energy per unit area (0.0065 W/m²) and the likely need for GHG intensive fertilisers [48]. Algae are able to achieve energy densities around 5 W/m² but necessitate the use of CO₂ rich ponds which would have to be derived from a low-carbon source such as crops thereby reducing their effective energy density [6].}
will be converted to biofuel plantations. This is not beneficial if areas of rain forest are destroyed which results in large quantities of GHG emissions, thereby increasing the CO$_2$ intensity of the resulting biofuel.

Given that the power consumption for global shipping is around 230 GW, this implies a land area of approximately $4.6 \times 10^5$ m$^2$, or roughly two United Kingdoms, would be required to grow biocrops. There will also be a variety of transport mechanisms also competing for biofuels that will have limited numbers of low-carbon options to employ besides biofuels, for example aircraft.

1.2.2 Hydrogen

Hydrogen is a potential low-carbon fuel for use in ships. Hydrogen is a crucial chemical product. Large quantities are needed in the production of ammonia (NH$_3$), mainly for fertiliser, and petroleum products$^3$. Consequently a way to produce hydrogen sustainably and with low CO$_2$ emissions is a very worthwhile goal. However, as an energy carrier it is plagued with various difficulties from production to distribution and storage to final energy conversion.

Production

Figure 1.4: The reactions that take place in the Iodine-Sulphur thermochemical process for producing hydrogen, along with the necessary temperatures. Whilst temperatures of around 850°C can be used to drive the process, it is preferable to utilise temperatures closer to 1000°C in order to improve efficiency (in terms of the energy content of the hydrogen created per unit energy input) [26].

$^3$By mass, ammonia ranks as the world’s fifth most produced industrial compound; the production of ammonia consumes around 2% of the world’s annual energy supply [3].
The majority of hydrogen (around 95%) produced for industrial use is via steam reformation of methane, that reacts high temperature steam (H\textsubscript{2}O) with natural gas (CH\textsubscript{4}) to result in H\textsubscript{2} and the greenhouse gas CO\textsubscript{2}. There is the potential for the CO\textsubscript{2} to be captured and sequestered, which is discussed in Appendix A.1. The remaining 5% of global H\textsubscript{2} production is via electrolysis [49].

Electrolysis is employed when hydrogen with very low impurities is required. The electrolysis process could be driven by a low-carbon power source; however, the efficiency of electrolysis (in terms of the energy content of the hydrogen created per unit energy input) is relatively poor when the energy losses in the production of electrical energy are also factored in (the net efficiency is around 25 to 35%) [50].

There is also the possibility of producing hydrogen in a thermochemical process at high temperatures as outlined in Figure 1.4. However, currently the necessary chemicals and temperatures create materials issues with respect to finding a vessel able to withstand the corrosive operating conditions [51], and whilst efficiency may be approximately double that of converting low temperature heat to electricity and then using the electricity to carry out electrolysis, the net efficiency is still relatively poor (around 50%) [49].

In order to supply the high temperature heat for the Iodine-Sulphur cycle it is necessary to employ a low-carbon heat source to ensure that the emission intensity is low. It is often assumed that [49] very high temperature reactors are employed in order to maximise the efficiency of the process. However, there are significant development barriers related to the deployment of Very High Temperature Reactors (VHTRs) [52]. Furthermore, VHTRs would perhaps be of better use serving the various industrial processes that would need to be decarbonised in the scenarios laid out in Figure 1.1.

Storage and Distribution

In order to store hydrogen once production has taken place it must be either sufficiently cooled to temperatures of around -250°C and/or compressed to around 600 atm\textsuperscript{4} [53]. Even once sufficient cooling and/or pressure has been applied the volumetric energy density for hydrogen is very low (around 1/6\textsuperscript{th} that of heavy fuel oil [43]). Therefore given that a large diesel powered container ship has a fuel tank that occupies around 2.5% of the total cargo carrying capacity [54], a hydrogen powered ship of similar size would require a fuel tank occupying around 15% of the cargo carrying capacity. This is a significant volume to dedicate solely to carrying fuel.

\textsuperscript{4}Hydrogen may also be stored physically, for e.g. by adsorption in spongy matrices of special alloys of metal hydrides or chemically in alkali metal hydrides, but to date this approach has not shown any advantages over cryogenic or pressurised tank methods [53].
There is also an associated energy cost for storing hydrogen in terms of the energy required to run the containment system as a percentage of the total energy content of the fuel. Currently the most efficient method (pressurisation) results in an energy cost of around 10% [50]. The low energy density also creates distribution problems as the produced hydrogen will need to be delivered for its final use, for example to the ship refuelling facility. Therefore, it would perhaps be more beneficial to locate the hydrogen production facility near to the ship refuelling facility to minimise distribution issues.

Conversion

In order to utilise the chemical energy stored in the hydrogen fuel a conversion system is required. This is usually performed using a fuel cell to convert the chemical energy into electrical energy to drive a motor. There are in general two types of fuel cells: low temperature (< 100°C) and high temperature (> 600°C) [55]. The low temperature fuel cells (such as the Proton Exchange Membrane fuel cell) utilise precious metal catalysts. However, their use of precious metals makes them very expensive and they typically have relatively low power outputs [43]. Hence, the preferred fuel cells for shipping applications are high temperature fuel cells which have the potential to be scaled to the necessary size to power large ships; however, currently these types of fuel cells suffer from a variety of material degradation issues due to their high operating temperatures [55].

Furthermore, the conversion process itself is also relatively inefficient having electrical efficiencies of around 50% [43]. When this is coupled with the 10% storage energy loss and the energy loss in producing the hydrogen (around 70% in the case of electrolysis) then for every unit of energy input used in producing hydrogen the electrical energy output from the fuel cell is only 0.135 units (or 0.225 units in the case of hydrogen produced via the Iodine-Sulphur cycle using VHTRs).

In conclusion, given the difficulty in achieving the levels of decarbonisation required in Figure 1.1, it seems prudent to attempt to utilise low-carbon energy as efficiently as possible. This is clearly not possible using hydrogen as the energy carrier. Hence, it would be preferable to find an alternative low-carbon fuel for shipping that is considerably more efficient than hydrogen and also has far fewer barriers to its deployment.

1.2.3 Nuclear

Nuclear power has been used at sea for almost 60 years after the first nuclear powered submarine, the USS Nautilus, was launched in 1955 [43]. This clearly demonstrates that in principle reactors can be
operated at sea on board a vessel of comparable size to a container ship. However, there are a number of distinct differences between naval and civilian vessels, namely the fuel materials they utilise and their operating histories. This results in the utilisation of naval reactors for civilian purposes being very low.

The vast majority of sea vessels that utilise nuclear reactors have been submarines. However, due to the classified nature of warships there is only some publicly available data on key parameters regarding power, capacity factors and fuel types. Firstly, the reported capacity factors for submarines (defined here as the average power output over the system’s life divided by its maximum power output) are very low (≤30%) [56, 57]. In addition, the maximum power outputs reported have also typically been less than approximately 200 MWth [56]. Finally, the fuels that have historically been utilised are so-called ceramic-metallic (cermet) fuels and metallic dispersion fuels such as U-Al and U-Zr [58].

Metallic dispersion fuels were created in order to overcome the many unfavourable characteristics of pure uranium metal (see Section 2.7.1 in the next chapter) by dispersing concentrations (less than approximately 50 wt.%) of fissile material in either aluminium or zirconium-based alloys [58, 59]. Cermet fuels on the other hand were created to overcome many of the disadvantages associated with UO$_2$ fuel (its brittle nature and very low thermal conductivity) yet still benefit from UO$_2$’s excellent behaviour under irradiation, its high melting point and low swelling rates [58, 60]. By dispersing ceramic UO$_2$ particles within a host metallic matrix this significantly improves the overall thermal conductivity of the material and greatly improves the mechanical integrity of the fuel. Russian submarine vessels have in the past apparently utilised a cermet fuel consisting of uranium dioxide particles embedded in an aluminium-based host material which is then clad in either stainless steel or zirconium [61].

Whilst metallic and cermet dispersion fuels are produced via different manufacturing processes they have a number of very similar characteristics. Furthermore, the fuel geometries for these fuel types have very high surface to volume ratios, such as plates [58, 61]. Together the fuel geometry and material type result in highly beneficial performance characteristics, namely:

5The reported power of aircraft carrier reactors are significantly higher than submarines (around 400 to 500 MWth [8]). Therefore assuming that the reactors are effectively derivatives of their submarine counterparts this implies that scaling up the power of submarine systems to produce maximum power outputs capable of powering large container vessels is a possibility. However, if aircraft carrier reactors’ capacity factors are comparable to submarines’ then they will also be of limited use for powering civilian systems.

6In principle fuel rod geometries could have high surface to volume ratios, assuming the rods can be manufactured to be sufficiently thin. In reality this would result in very fragile core fuel elements and therefore they have typically not had rod thickness less than approximately 0.90 cm [16].
Both cermets and metallic dispersion fuels have very high thermal conductivities;

Thin plates result in low centreline temperatures and low surface heat fluxes;

A fuel material with a similar thermal expansion coefficient to the clad material. This is particularly beneficial during power increases where if the thermal expansion coefficients were considerably different then one material will expand faster than the other. This would result in stresses accumulating at the boundary between the fuel and clad, increasing the likelihood of failure occurring.

The first two points result in the fuels having low centreline and surface temperatures, which minimises a variety of fuel degradation mechanisms, such as chemical attack from fission products, oxidation of clad surface (which is temperature dependent) and mechanical stresses due to thermal expansion. Finally, the fuel forms also minimise the migration of fission products from the fissile components of the fuel to the clad, as the migration of fission products to the clad surface is impeded by the host material. All of these properties result in very robust fuel forms with high mechanical integrities and fission product confinement. This permits a reactor core utilising these materials to undergo large variations in power output over very small time periods at very high burnups (>> 60 Gigawatt-days per tonne of Heavy Metal (GW.d/tHM), where the term heavy metals refers to elements with atomic numbers greater than actinium). However, there are considerable economic penalties that result from such a fuel form. Firstly, the manufacturability of such fuel is more complex than the conventional UO$_2$ pellets clad in zirconium-based tubes. In addition, the fact that a significant fraction of the fuel volume ($\gtrsim$50%) consists of non-fissile materials, results in the need to utilise highly enriched uranium if a long core life is required and the overall core volume is small. The use of highly enriched uranium is not only economically unfavourable but also prohibits the use of these fuel forms for civilian applications (see Section 2.2 in the next chapter).

It should be noted that when designing a military vessel the primary aim is to create a system with excellent performance characteristics. This is because the vessel must be able to carry out its various duties without prohibitive restrictions on the power variation of the core due to limitations

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7 French naval reactors utilise a unique plate fuel concept (called Caramel which is discussed in the next chapter) which is significantly less robust than cermet and metallic dispersion plate fuels.

8 As dispersion fuels have a number of components (the fissile material, the host material and the clad) this results in greater complexity relative to a fuel material that consists of only fissile and clad materials. Furthermore, it is important that the host and fissile materials are homogeneously mixed in dispersion fuels which results in more checks required during manufacturing relative to non-dispersion fuels. Finally the clad must be bonded to the fuel material and analysed to ensure sufficient bonding has taken place.
imposed by the materials employed. In the case of a civilian nuclear powered vessel the operating regime, and therefore the priorities, are likely to be very different. For instance, a civilian vessel will need to frequently enter ports potentially in close proximity to high population centres, and also have to navigate waters where there is a non-negligible risk of collision with other ships. In addition, a nuclear powered civilian ship will have to be competitive with other low-carbon fuel forms. Hence, a strong emphasis arises regarding safety and economic characteristics.

Besides naval vessels there has been some experience operating what could be termed civilian nuclear powered vessels. Russia has deployed a number of nuclear powered icebreakers, although historically they have utilised a cermet fuel using highly enriched uranium [8, 64]. However, future icebreaker cores are reported to use fuel enriched to less than 20 wt.% $^{235}$U but this is also a cermet fuel type that will apparently use a zirconium-based alloy host material embedded with UO$_2$ particles [65]. Furthermore, the reactor will have a relatively low maximum power output of 174 MWth, a low capacity factor (around 65%) and require refuelling every 7 years [66], thus making it of limited use for a civilian container ship (see Section 2.4 in the next chapter).

More conventional reactor types, i.e. that utilised low enriched uranium cylindrical fuel rods containing UO$_2$ pellets, have been deployed at sea; these are listed in Table 1.3.

<table>
<thead>
<tr>
<th>Ship name</th>
<th>Power</th>
<th>Enrichment</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mutsu</td>
<td>36 MWth</td>
<td>5.8 wt.%</td>
</tr>
<tr>
<td>NS Savannah</td>
<td>74 MWth</td>
<td>$\sim$4 wt.%</td>
</tr>
<tr>
<td>Otto Hahn</td>
<td>36 MWth</td>
<td>$\sim$5 wt.%</td>
</tr>
</tbody>
</table>

Table 1.3: List of civilian nuclear powered ships that have utilised fuel similar to that found in large commercial reactors [8]. The Russian Sevmorput nuclear cargo ship has not been included here as it uses highly enriched fuel [8].

All of the ships in Table 1.3 were in service for approximately 10 years [8, 67]. The highest powered of these vessels, the Nuclear Ship (NS) Savannah, travelled in total 450,000 nautical miles and undertook one partial refuelling during its lifetime of 10 years [67]. However, whilst nuclear powered ships have operated successfully in the past, in Section 2.4 in the next chapter a case is made for wanting to increase the refuelling period to once in a container ship’s typical 30 year lifetime [1] rather than once every 5 years. In addition, the power outputs from the cores would have to be significantly increased from less than approximately 75 MWth to around 400 MWth (see Section 2.3). In order to achieve these goals it was decided to investigate the feasibility of employing conventional

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9Both cermet and metallic dispersion fuels have very favourable safety characteristics due to their highly robust nature but the economic penalty in achieving this is high.
LWR technology (defined in the next chapter) which should minimise the barriers, and therefore the
time required, to deploy nuclear reactors in the shipping sector.

Most published work regarding nuclear powered ships has focused on the benefits and challenges of
nuclear powered vessels relative to alternative low-carbon fuels [43, 25]. A few recent studies have been
performed regarding non-core specific design work such as the integration of a nuclear reactor and its
coolant system into a large ship [68, 69, 70]. There has been very limited (if any) work performed
relating to 3D core design for a reactor capable of powering large ships and achieving high capacity
factors (\(> 80\%\)) without the need to refuel for time periods significantly greater than 5 years.

As the vast majority of reactors that have been deployed at sea have been PWRs we have decided
to focus on developing a PWR core specifically designed to power large container ships. This is mainly
because there is a far greater wealth of information regarding operation of PWR systems at sea as
discussed previously.

It is worth mentioning that there are a number non-technical barriers with regards to deploying
nuclear powered civilian vessels. Firstly insurance presents a considerable problem. There is currently
insufficient actuarial data to accurately determine the risks associated with operating nuclear powered
container ships [43]. This results in a large degree of uncertainty with respect to ensuring sufficient
finance is in place to cover the costs associated with any accident. Whilst there are operating PWRs
on board ships at sea, these do not operate under the same conditions as container ships namely:
frequently visiting ports near high population centres and travelling in busy ship lanes where the risk
of collision is not negligible. Whilst oil companies are able to obtain insurance for their large oil
tankers vessels, which can experience very severe accidents, for example the Exxon Valdez Oil Spill
which is estimated to have cost, in 2010 dollars, around $7 billion [71]. However, it is important
to note the differences between the balance sheets of very large oil companies such as Exxon Mobil,
with annual operating incomes of around $40 billion and total assets of $350 billion compared with
operating incomes of around $10 billion and total assets of $65 billion for Maersk, the world’s largest
operator of container ships. Therefore, if the insurance costs were comparable to insuring a large
oil tanker this may prove prohibitive for the operator of a container shipping company. In order to
reduce the economic risks to the operator of the ship it may be necessary to insist on government, or
governments, to underwrite the insurance, as is currently the case for conventional land based nuclear
power plants, where the operator’s liability is typically limited to around £1 billion, and beyond this
limit the state acts as insurer of last resort [72].
Port restrictions are also likely to be in place as a number of countries are opposed to nuclear power and may not permit the vessels to enter their waters. However, the overall effect will likely be limitations with respect to the route a nuclear powered ship can take (see Section 2.4 in the next chapter).

Disposing of nuclear waste will also perhaps be more complex than for waste produced at land based systems. This is because whilst the operator will likely have to cover the cost of disposal it will be necessary to find a country willing to host the nuclear waste. There is currently opposition within many countries regarding for disposal of nuclear waste from land based system even when those countries have benefited for decades from the low-carbon electricity their reactors have provided [52]. Hence, if the ship has served a number of countries in transporting goods, should the waste therefore be split between those countries or should the operator come to some sort of arrangement with their own country to deal with the waste?

Another potential issue will be the need and costs associated with well-trained staff able to operate a nuclear reactor on board a ship and issues regarding safety from say collisions, foundering and grounding of the ship. Yet there may be a role for technology to alleviate these issues and they are discussed in the next chapter and the conclusion of this report. However, it is worth noting that not all vessels will be suitable for the deployment of nuclear reactors as even small reactors have a relatively large footprint once shielding, pipework and the containment vessel have been factored in. This footprint may extend to roughly 3000 m$^3$ [73] and therefore probably only the larger ship types outlined in Figure 1.2 would be suitable for nuclear power, namely some types of container ships, passenger vessels, bulk carriers and tankers.

1.3 Summary

There will undoubtedly be some difficulties in the implementation of nuclear power for civilian ships including, but not limited to, a number of non-technical barriers relating to insurance and responsibility for the waste. However, the necessary carbon reductions outlined in Figure 1.1 and the fact that other potential fuel sources have considerable drawbacks suggest it is worthwhile investigating the feasibility of powering at least some vessels with nuclear reactors.

Given that the emissions from container ships are likely to dominate future shipping emissions, and the size of some container ships makes them suitable for implementing small reactors on board,
it was decided to study the feasibility of nuclear powered container ships.
Chapter 2

Parameters

2.1 Requirements, Goals and Limitations

The primary aim of this investigation was to work out whether it was possible to power a large container ship, for an extended period of time, using conventional Light Water Reactor (LWR) technology. However, before starting to develop a viable reactor design it is important to set out the various demands there will be on the system, and thus define the parameters. In addition, it is necessary to determine their relative priority; this was achieved by considering the parameters in terms of requirements, goals and limitations. The Requirements are highly important physical or performance features that should be present in the final design, and in some cases are hard constraints that must be obeyed. Goals on the other hand are features that are determined to be desirable but are not believed to create any major obstacles if they were not present in the final design. Limitations are constraints that are imposed on the investigation, which tend to reduce the number of free variables and can help achieve the final design solution more quickly.

2.2 Enrichment

An overriding requirement is that because this reactor is to be used in a civilian setting, the reactor cannot use highly enriched uranium, that is uranium with an enrichment greater than 20 wt.% $^{235}\text{U}$. This is a globally agreed limit whereby enrichment below this level has been deemed to present limited proliferation concerns, primarily because the unmoderated critical mass below 20 wt.% is so large that
it is not possible to produce a viable weapon design [74, 75].

2.3 Core Power

As discussed in the previous chapter, there has been a tendency for ships to become larger in order to benefit from economies of scale as each ship can carry more cargo, thereby reducing costs associated with transporting each container on board the vessel. Therefore, it was considered appropriate to study recent engine designs capable of powering large container ships, as an indicator of the power the reactor needed to produce.

Two of the biggest producers of diesel engines for large ships are MAN Diesel and Wartsila, and together they dominate the market share in the marine engine propulsion sector [76]. Their largest engines built to date for container vessel propulsion are the 14K98MC MAN engine capable of outputting 79 MW, and the Wartsilla RTA96C engine producing up to 80 MW [77, 78]. Given that propulsion usually makes up around 75% of ship power requirements, with the other 25% being referred to as hotel load - referring to power requirements for refrigeration, navigation and crew amenities - the total power requirement for the reactor studied in this work has been set to 110 MWe [79]. It has therefore been assumed that the reactor will produce electricity rather than powering the propeller directly simply because the hotel load is quite substantial; therefore a large amount of electricity will need to be produced in the first place. Also, by permitting the reactor to produce electricity it increases the flexibility in reactor operation. For instance, when the ship is in port the reactor could in principle be connected to the electrical grid and generate power, or it could be used to charge batteries that may act as a backup for various systems on board.

2.4 Core Life and Capacity Factor

Modern ships typically have lives of around 30 years [1]. Over this 30 year period they undergo routine maintenance during dry docking which currently takes place every 5 years. However, there is the possibility that this will be expanded to 7.5 years in the near future due to the economic cost of taking ships out of service [80].

Refuelling a reactor on board a ship is unlikely to be as rapid as the targeted refuelling period of less than 20 days large PWRs are able to achieve [81]. This is because large PWRs are designed
to be flooded and a crane is already inside the containment building that can readily transfer the individual assemblies from the reactor building to the spent fuel pond. It was decided therefore that even if refuelling does require a longer dry docking period than is normally the case, this would still be acceptable if refuelling the core is performed on a relatively infrequent basis. In addition, it is likely that ports able to refuel nuclear powered ships will be very limited in number and expensive to operate. Therefore the greater number of ships each port is able to service, the lower the economic penalty. Also, with any type of reactor there is the possibility that the time taken to refuel may take longer than was expected due to some unforeseen circumstance. Therefore, if ships are able to run slightly longer than their targeted core life, any scheduling conflict in port will not cause ships to become ‘mothballed’ whilst they wait for a port to become available. All of these points lead to a strong motivation to study the maximum achievable core life. It was assumed that it would not be possible to design a nuclear reactor using well established materials capable of achieving a core life of 30 years because various degradation mechanisms, such as corrosion, would render the reactor inoperable long before the 30 year core life was achieved. However, it was thought that a 15 year core life would perhaps be achievable. A 15 year core life is easily accommodated with current and potential dry docking periods every 5 or 7.5 years, and also means that each ship would only need to undergo refuelling once during their lives.

For pragmatic reasons it has been assumed that the core would operate on roughly a 23 day cycle, of 3 weeks at full power whilst travelling between ports and 2 days in port for cargo loading. The reasoning behind this assumption was that it appears unlikely that nuclear powered ships will, at least initially, be permitted to operate in exactly the same manner as conventional ships due to the fact that a number of countries are likely to place restrictions, for political reasons, on nuclear vessels entering ports\textsuperscript{1}. Furthermore, even if a large number countries did permit vessels, it will likely be necessary that the reactor design is licensed in each country the ship enters before it could complete its voyage. Therefore, if for instance a ship enters say around a dozen ports during its normal operation (as is usually the case [82]), it will currently have to gain certification from each of the countries nuclear regulators before it can operate that particular route (a likely expensive and time-consuming process). For these reasons, it appears likely that a ship will operate between a smaller number of ports and therefore undergo less frequent port visits but reside longer in port in order to unload and load a

\textsuperscript{1}Large ships typically operate on a schedule of approximately 4 days between ports and less than 24 hours stationed at a port [82].
larger proportion of its cargo capacity.

The Capacity Factor (CF) was simply determined by assuming that the power level in port is reduced to the hotel load (around 25%) and when at sea it is travelling at full power, hence a CF of 93.5%. This value is conservatively high for a number of reasons. Firstly, looking at a 9 month segment of the Emma Maesrk schedule (one of the largest container ships in operation) returned a CF of 85% [82]. In addition, during the 15 year core life the ship will undergo some dry docking for maintenance, further reducing the CF. Nonetheless, it seemed sensible to overestimate the CF of the reactor by a relatively small margin as it inherently makes the calculations more conservative, especially when considering fuel performance, which is highly dependent on burnup. In addition, a higher CF will lead to conservative estimates of the minimum enrichment required to operate the system for the targeted core life.

2.5 Reactor Geometry

The largest cargo vessels typically have lengths, widths and hull heights of around 400 m, 60 m and 30 m respectively [79]. The diesel engine alone can have dimensions of 26 m in length, 13 m in height and 7.5 m in width, weighing 2300 tonnes [83]. Therefore, there is significant space on board for a reactor. However, there are clearly benefits to keeping the reactor as small as possible, not least because it permits more space for cargo to be stored and therefore allows greater operating revenues. It must also be factored in that there would be significant space demands for the Steam Generators (SGs), pressuriser, shielding and containment (an ordinary ship hull would not constitute a nuclear containment barrier in the conventional sense), nevertheless a smaller reactor would reduce the footprint of the entire nuclear steam supply system.

In recent years, so-called Small Modular Reactors (SMRs) have gained interest. The primary aim of these systems is to reduce the size of the reactor in order to reduce the capital cost to the extent where it becomes favourable for certain sectors to consider investing in nuclear power (many sectors cannot afford or require >1 GWe plants as is the case in the shipping sector) and also to benefit from economies of mass production rather than economies of scale. The latter point is highly uncertain as usually there are a number of essentially fixed costs in building a nuclear power plant, for instance licensing the reactor and securing the facility, therefore specifying a larger power reduces the relative expense of these costs. Furthermore, for many reactor components it may be the case that
their price does not scale directly with the power output [84]. However, there are benefits that may offset some of these disadvantages, for example by taking advantage of the smaller size it may permit new reactor designs and manufacturing methods to be used. An example of this is so-called integral reactors, whereby the steam generators and pressuriser are placed inside the reactor pressure vessel [85]. The main benefit of integral systems is that they eliminate various scenarios that could result in a ‘large-break loss-of-coolant accident’ (LOCA) such as a pipe rupturing between steam generators and reactor pressure vessel. Constructing an integral system is not possible with large reactors, as the size of a conventional Reactor Pressure Vessel (RPV) is already very large and incorporating the SGs and pressuriser (in themselves both very large components) into the RPV is, from a manufacturing standpoint, prohibitive [85]. This is much less of a problem for smaller systems.

Small modular reactors typically have RPVs with diameters of less than around 3.5 m [86]. The reasoning behind this designated RPV size is simply because there are a larger number of suppliers able to produce steel forgings of this size, whereas there are very few companies currently able to produce the ultra-large forgings required for conventional PWRs. Therefore there is an expected reduction in the cost of producing these smaller RPVs as demand can be more easily met [85]. Given that there are arguments for designing a core to fit inside a 3.5 m envelope and there are a number of companies with mature designs and capabilities in designing licensable reactors with this size, it seemed practical to set 3.5 m as a goal.

2.6 Eliminating Soluble Boron

There is considerable uncertainty about the feasibility of being able to license a nuclear powered ship with a limited number of personnel on board. For example, a large cargo ship typically has around 12 members of crew compared to around 100 on board a submarine [79, 87]. However, a nuclear powered submarine is significantly more complex than a large cargo ship, as, apart from the addition of a nuclear reactor, the submersible vessel also contains atmospheric regeneration systems, multiple weapons systems and high precision navigation systems. Nevertheless, it is prudent to try to identify systems that add to the complexity of the reactor system and whose removal may significantly simplify reactor operation. A particular focus was given to systems that directly influence neutronics and fuel performance given the scope of this investigation. A key system identified was the system that delivers and maintains the correct concentration of Soluble Boron (SB).
Soluble boron is utilised for reactivity control in PWRs, by adjusting the amount of boron in the reactor coolant and therefore the relative concentration of $^{10}\text{B}$, which has a thermal neutron absorption cross-section of 3800 barns [88]. The benefits of SB are:

- SB reactivity control is, in principle, diverse from the control rods$^2$;
- Allows more uniform core power profiles;
- Easily compensates for the initial high reactivity of the fuel at the beginning of life.

For large reactors it also has the considerable benefit of improving uranium utilisation by permitting the amount of poison present in the core to be finely adjusted throughout core life, thereby relying less on solid burnable poisons in the fuel. This reduces the mass of fuel within the core and also significantly reduces the residual poison concentration, that is to say the extent to which any remaining (residual) poisons at the end of cycle reduce the achievable cycle length [88]$^3$. However, in the system being studied here it was envisaged that a number of benefits relating to:

1. Economics;
2. Safety;
3. Radioactive waste;
4. Effects of soluble boron on corrosion;

would outweigh the primary benefits usually attributable to SB. Furthermore, a technical feasibility study performed by Combustion Engineering (CE) for the Electric Power Research Institute (EPRI) into the elimination of SB for large PWRs came to the conclusion that [88]: “A significant result of this study is the realisation that the feasibility of a soluble boron free design improves as the core power and size are reduced, primarily because of the intrinsic xenon stability of small PWRs$^4$. Further, current

$^2$Diversification is one of the means to improving the performance of a safety function, and thereby reduce the likelihood of system failure. For instance, if the mechanical system (e.g. control rods) for shutting down a reactor fails, then a chemical system that is independent of the control rods should improve the likelihood of the function required (reactor shut down) being successfully carried out in comparison to only one system being in place.

$^3$In the case of a reactor which relies entirely on soluble boron for reactivity control, there is no residual poison penalty as the poison concentration at the end of life can become effectively zero through dilution. Although in reality some solid burnable poison is always present to at least provide more uniform core power profiles.

$^{135}$Xe has a very high thermal absorption cross-section (2.7 Mb) and can therefore heavily influence the thermal flux within a region of the core. Furthermore, the inventory of $^{135}$Xe exhibits time dependence as its production and loss depends on the half-lives of both $^{135}$Xe and its parent nuclides. This therefore creates the possibility for localised variations in $^{135}$Xe concentration within the core, which can lead to so-called xenon oscillations. These oscillations can dramatically increase the power within certain regions of the core and may thus result in fuel failure. However, xenon oscillations tend to become more pronounced for cores with large linear dimensions [89].
thinking on small PWRs generally tends towards lower average power density than existing large PWRs, allowing the former to more easily accommodate the higher relative power peaking expected in any soluble boron free design.”

Therefore, any benefits attributable to a Soluble Boron Free (SBF) design should be particularly pertinent to the small, low power density core designed in this study. However, by eliminating or at the very least reducing the extent of SB requirements, it was expected to considerably complicate core-design. This is due to power peaking creating issues relating to fuel performance, as certain rods within the core will experience much higher duties and so will suffer more from various degradation mechanisms. Therefore, given that there are distinct drawbacks to operating without SB, it seems important to discuss in some detail the relative advantages and disadvantages associated with an SBF design.

2.6.1 Economics

The SB system is a considerable chemical plant and is incorporated into the Chemical Volume and Control System (CVCS) in most nuclear power plants. The CVCS’ primary aim is to purify the reactor coolant and maintain favourable chemical conditions that limit corrosion by the addition of corrosion-inhibiting chemicals [90]. The addition of the SB system into the CVCS requires the addition of a number of large tanks, heat exchangers, pumps, piping, valves and control systems for the mixing and delivery of the desired boron concentration to the reactor coolant system [91, 92]. In order to make alterations in boron concentration a temperature-dependent ion exchange resin is employed, which at low temperatures (around 10°C) absorbs boron, and at higher temperatures (around 60°C) releases boron into the reactor coolant [93]. This system, referred to as the Boron Thermal Regeneration System, operates at low temperatures and pressures, which are very different to the primary cooling circuit conditions of high temperature and pressure. Thus, systems are required to cool and depressurise the coolant for entry into this part of the CVCS and then to subsequently raise the temperature and re-inject it into the primary circuit. For these reasons it is believed that by removing the SB control system from the CVCS, considerable plant simplification can be carried out, in particular a closed loop, high-pressure coolant purification system would probably be used [88].

Soluble Boron Free (SBF) operation also offers enhancements in the operation of the nuclear sampling system as less frequent samples are required to be taken [92]. This is perhaps a considerable advantage with respect to keeping the system simple in order for it to operate on a civilian ship with
limited personnel to carry out sampling and to analyse the coolant chemistry. A further complication with the addition of SB is that the systems that carry boron must be heated in order to avoid crystallisation and the formation of solid deposits that would build up and cause blockages [91]. This further adds to the cost of pipes and tanks containing SB. Another advantage related to SBF operation is an increase in flexibility as power variations are limited, particularly later in core life, by the dilution time [92]. SBF operation could allow for a gain in operational flexibility which is important in marine applications where the core will be expected to increase and decrease power upon leaving and entering ports.

Given the reliance on control rods as the main mechanism for reactivity control throughout life, it was assumed that the design of an SBF reactor would necessitate a greater number of control rods than in a conventional reactor. This is disadvantageous with respect to economics as the hardware that is associated with driving control rods into the core - the Control Rod Drive Mechanisms (CRDMs) - is relatively expensive [88]. In addition, as they carry out a very important safety function, this necessitates that each drive has associated with it control and sensor cables that must be routed to the control room, whilst also meeting stringent requirements on isolation, fire protection and containment penetrations [88]. However, Boiling Water Reactors (BWRs) usually have control rods (technically referred to as control blades) in every fuel assembly and therefore any extra cost attributable to an increase in CRDMs is not believed to be prohibitive or reduce the net benefits when factoring in the above economic advantages.

2.6.2 Safety

There are a number of safety advantages attributable to a reduction or total elimination of SB. A reduced (more negative) Moderator Temperature Coefficient (MTC) throughout core life is often quoted [88, 91, 92]. However, there are advantages and disadvantages associated with a reduced MTC.

With respect to the advantages, it is certainly the case that as most accident scenarios involve the impairment of core cooling, such as loss of feed water or primary coolant flow, and therefore result in temperature increases in the reactor, a more negative MTC will be beneficial [92]. This is because the consequences of temperature increases are reduced as greater amounts of negative reactivity are inserted into the system in these events. However, whilst this is favourable, it is usually not limiting in reactors that utilise SB. A more important characteristic is that the fuel is always covered with coolant and by removing the requirement for SB and therefore reducing a number of pipes, this would
reduce pathways for loss-of-coolant accidents to arise. Furthermore, the low power density of such a system, which is typical of SMRs but unrelated to SBF operation, has the advantage of increasing the relative inventory of primary coolant. This latter point will prove of greater significance than a reduced MTC [88].

Whilst most accident scenarios involve core temperature increases, there are some cases where a more negative MTC is potentially unfavourable. For instance, in the event of rapid core cooling, caused by for example the inadvertent opening of a secondary relief valve or a main steam line break, will result in an increase in reactivity. It is therefore important to ensure there are strategies in place that can ensure that sufficient negative reactivity can be inserted that can counteract any increase in reactivity as the core rapidly cools, e.g. appropriate control rod worth. It is necessary that in an SBF design this is guaranteed, and therefore constituted one of the characteristics the SBF core designed in this study was measured against. Furthermore, in the cases where control rods alone cannot guarantee sufficient negative reactivity, as is the case in conventional PWRs, then the onus turns to the SB system to compensate for the increase in reactivity [92]. Thus there would be a net benefit due to a simplification in management response for this particular transient type. Assuming control rods are able to counteract rapid core cooling, then overall a more negative MTC will be beneficial.

So far the benefits of reduction or elimination of SB are on balance beneficial from a safety perspective, although they are likely to be of secondary importance compared to the unrelated benefit of a greater coolant inventory typical of most SMR designs. However, there is one class of accidents where the reduction or elimination of SB is very favourable: inadvertent boron dilution.

Boron dilution accidents are characterised in terms of homogeneous and heterogeneous accidents. Homogeneous dilution accidents are considered in conventional PWRs to be a relatively common occurrence (around $10^{-2}$ per year [94]) but they operate on relatively long timescales, therefore giving time for countermeasures to be initiated that may effectively neutralise the transient. Much of the prevention relating to homogeneous boron dilution is procedural, with protection focused on automated systems that are in place to detect anomalous boron concentration and then initiate necessary countermeasures, such as automatically increasing boron concentration. Homogeneous dilution scenarios include operator error, such as simply reading a dial wrong and over diluting, as well as sudden and random startup of systems that dilute the reactor coolant.

Heterogeneous dilution events are considered much less likely than homogeneous dilution events
but can cause severe core damage. They are characterised by the formation of a concentrated volume of unborated water (a slug) entering the primary circuit, whilst the boron concentration in the rest of the reactor coolant system remains unchanged [95]. Therefore the reactivity insertion associated with heterogeneous dilution events can take place on a much shorter timescale than homogeneous events. An example of a heterogeneous dilution that can occur is when the water level in the reactor coolant system is low and water begins to boil. The steam produced can then flow towards the steam generator tubes and condense, thus turning into unborated water [96]. The unborated water can then enter the region surrounding the Reactor Coolant Pumps (RCPs). If the RCPs were then to be restarted, say to reenable cooling of the core after a loss of power, this slug of unborated water could then be transferred to the core with initially little mixing taking place, causing a criticality accident. If the slug is sufficiently large then the reactivity insertion could be sufficient to cause severe core damage [94]. In addition, by removing or reducing the need for SB then the negative consequences related to heterogeneous dilution by Steam Generator Tube Rupture (SGTR) are greatly reduced [92].

Firstly, as the SGs operate at lower pressure relative to the primary circuit (70 atm vs 150 atm), the pressure needs to be rapidly equalised in order to limit the extent of loss of reactor coolant from the primary circuit, with the SG then isolated from the remainder of the secondary circuit. Therefore, there is the risk that any unborated water present in the SGs could lead to a heterogeneous dilution accident once the pressure is equalised. Secondly, the SG safety valves are normally located outside the containment building in order to limit dilution events occurring within the containment structure, as the SGs naturally contain unborated water. The downside of this strategy is that it creates a pathway for external release of activated coolant, as in the event of an SGTR, activated coolant may now reside within the SGs. Consequently, if the core is cooled with unborated water then there is no risk of dilution and thus SG safety valves can be located inside the containment structure [92].

If it is possible to develop a licensable design that is able to achieve satisfactory core cooling, in any reactor state, with unborated water alone, then there is likely to be the considerable advantage in giving greater flexibility to operators in accident scenarios. This is because there would no longer be any concern related to maintaining sufficient boron concentration within the primary circuit and therefore any reserve containing unborated water can be used to keep the core cool. In addition, in the event that these reserves are not available, the operator could turn to using sea water to cool the reactor as a last resort. This is not preferable as salt water is corrosive to reactor internals and the reactor would be of no further economic use. However, as a method of last resort it is clearly
preferable to allowing the accident to propagate further without satisfactory quantities of coolant.

In Ref. [88] it was believed that an soluble boron free PWR would still require an Emergency Boration System, as is the case for BWRs. The Advanced Boiling Water Reactor (ABWR), which is a BWR variant designed by GE Hitachi, has a Standby Liquid Control (SLC) system that is able to inject sufficient soluble boron to shutdown the reactor from any state with no control rod motion and maintain the reactor in a sub-critical state at room temperate (≈ 20°C), with a considerable safety margin [97]. However, the SLC system is a relatively slow means to achieve shutdown, taking up to 10 minutes for sufficient boron to be injected in order to keep the reactor shut down for all conditions. 10 minutes is a relatively long time frame in comparison with a successful scram, that is able to shut the reactor down in around 3 seconds [97]. However, this time could be reduced given a sufficiently high concentration of $^{10}$B.

Another significant advantage of an SBF design is the disappearance of a phenomenon referred to as the Axial Offset Anomaly (AOA). The Axial Offset (AO) is defined as the difference in power between the top half of the core and the bottom half of the core, divided by the total core power. Therefore, the AOA is simply a significant deviation of the Axial Offset in the operating core from the predicted axial offset, where ‘significant’ is typically taken as a core-wide deviation of more than 3% [98]. For the AOA to occur three conditions are necessary: sub-cooled nucleate boiling (that is, localised boiling on the rod surface but with the bulk coolant temperature still below the saturation temperature), sufficient deposition of corrosion products and a sufficiently high boron concentration. These three phenomena result in a porous deposition of corrosion products developing, with a high concentration of boron present within the porous structure. As sub-cooled nucleate boiling preferentially arises in the top portion of the fuel, this can lead to an asymmetrical distribution in boron along fuel channels, resulting in a suppression of reactivity in the top portion of the reactor, thus leading to the AOA.

The most severe consequence of an AOA is a decrease in shutdown margin, resulting in impairments to safety characteristics of the core design. Other disadvantages include economic costs, due to necessary reduction in power required to recover an adequate shutdown margin, and increase complexity for crew to manage the AOA [98].

The AOA was only noticed, on any significant scale, in the late 1990s, as reactor coolant temperatures were increased and therefore many of the processes required for the onset of the AOA - namely corrosion and sub-cooled nucleate boiling - more readily take place. Given that there are strong economic drivers for these higher coolant temperatures, it has not been possible to eliminate
the occurrence of the AOA by reducing coolant temperatures. Therefore, to date, procedures are put in place to try to limit the occurrence of the AOA, such as improved water chemistry control and reduction in power peaking [98]. However, with an SBF design the Axial Offset Anomaly does not arise in the first place.

There is potentially the significant drawback that by relying heavily on control rods to compensate for reactivity changes over core life to ensure safe shutdown, this would adversely impact the effects of control rod ejection. This is because the greater required rod worth implies a larger reactivity increase in the event a control rod is rapidly removed from the core. Therefore, another criterion was put in place for the core being designed here: that the reactivity increase during rod removal must not be large enough to permit the core to become prompt critical (see Section 3.3.3 in Chapter 3 for a more detailed discussion on this criterion).

Whilst the extent of SBF operation has little direct bearing on core design, and the fact that the multitude of accident scenarios are beyond the scope of this investigation, it does impact the magnitude of benefits associated with an SBF design. As discussed above, and also concluded in Ref. [92], the benefits attached to SBF become more significant the greater the extent of SB elimination. This hinges crucially on whether it is possible to design a sufficiently diverse and redundant means to ensure safe shutdown and in the event that core degradation (melting) occurs, that unborated water is sufficient to ensure no return to criticality. In addition, the shutdown system would need to prove its operation is simple and cheaper than using boric acid to control reactivity in accident scenarios. These matters are discussed further in the conclusion of this study.

### 2.6.3 Radioactive Waste

The majority of the tritium in a reactor comes from ternary fission in the fuel rod. However, tritium produced within a fuel pellet is usually retained within the fuel rod as Zr has a high affinity for hydrogen. Therefore, almost all of the tritium within the coolant is not from ternary fission but due to high energy neutrons interacting with $^{10}$B in the coolant resulting in the production of tritium [99]. Consequently, removing boric acid will reduce doses to personnel by reducing tritium concentrations and by reducing the number of circuits that transport primary coolant, which results in less required maintenance work [92].

The ion exchange resins in conventional reactors also experience quite high duties (when boron is present in the coolant) in comparison to other components in the CVCS and therefore require regular
maintenance. As they need to be replaced quite frequently, this creates a waste stream that would be significantly reduced in an SBF design [88]. There is also the economic advantage of reducing this waste stream and also reducing maintenance requirements.

### 2.6.4 Effects of Soluble Boron on Corrosion

Boron normally plays the important role of inhibiting the penetration of lithium (Li) in the clad oxide layers that form, thus reducing the cladding corrosion benefits of an SBF design [92]. In view of the operational restrictions on the oxide thickness of the cladding, concerns that SBF operation could be disadvantageous if pH is controlled by lithium hydroxide alone arise. However, this is unlikely to prove a major obstacle to the deployability of an SBF reactor given that CANDU systems have made use of conventional clad materials and do not operate with SB; this is discussed in more detail in Section 2.7.3.

Besides this potentially small disadvantage associated with the reduction in SB there is likely to be considerable benefit in reducing or eliminating boric acid induced corrosion. Boric acid induced corrosion typically occurs due to a leak that results in the coolant flashing from a liquid to steam due to the sudden pressure drop. This results in a concentrated boric acid solution, which can corrode the carbon steel components if there is no method for detection or mitigation of the problem [100].

In the US, boric acid induced corrosion has resulted in a number of incidents that led to the degradation of the primary pressure boundary, which could result in a serious loss of coolant accident. Five events in the 1980s, that ranged from corrosion damaging components related to the coolant injection systems, to boric acid corroding a valve resulting in 70 cubic metres of reactor coolant entering the containment building, led to the US Nuclear Regulatory Commission requesting assurances that procedures were put in place to ensure that similar incidents were highly unlikely to occur again [101]. Nevertheless, in 2002 a potentially serious incident was narrowly avoided when boric acid induced corrosion led to severe degradation of the reactor head cavity at the Davis-Besse plant in Ohio. During a planned refuelling outage it was noticed that a section of the reactor vessel head had corroded to such an extent that only a thin layer of material (approximately 0.95 cm) was left to stop the primary coolant from escaping. As a result of the corrosion that took place at the Davis-Besse plant, a whole generation of reactor vessel closure heads were replaced [100]. The closures were replaced with Alloy 690 reactor vessel penetrations as opposed to Alloy 600 due to 690’s known superior corrosion resistance, and the weld filler materials were also altered [102]. Numerous other
boric acid induced corrosion incidents have been recorded in PWRs; see Ref. [100] for more details.

The above events highlight the importance of routine inspection to examine and evaluate locations where leakage is likely to occur and the detection of small leaks that are precursors to many of the incidents that have followed [101]. Therefore, by eliminating, or reducing the need for SB during most operation conditions, there would be a significant benefit in either ruling out or decreasing the likelihood of boric acid induced corrosion. It has been suggested that in fact this may be the single greatest benefit of SB elimination by reducing the long down-time following primary leaks [88]. Without boric acid, the cleanup following leaks is much easier, as the coolant activity is greatly reduced by removing a pathway to tritium production. In addition, inspections and evaluation of boric acid induced corrosion are not necessary, which is particularly relevant when trying to design a reactor system that is capable of being safely operated and maintained by the limited number of personnel on board a ship.

2.6.5 Final Remarks on Soluble Boron

Many of the net benefits associated with eliminating soluble boron exist even in the event that the reactor only operates without soluble boron during normal operation, i.e. in events that exclude certain accident scenarios. However, if it is assumed that soluble boron may be injected into the reactor coolant system under particular off-normal (accident) scenarios, then this significantly increases the number of constraints relative to a system that completely eliminates any need for SB. For example, under normal operation many of the circuits would not contain soluble boron, but once a particular accident has been initiated that requires the injection of SB these systems must be isolated from the reactor coolant system in order to ensure that any unborated water within these circuits does not end up diluting the boron within the primary coolant. This not only complicates the management of an accident but will also limit available reservoirs that can be called upon to ensure adequate coolant, including the sea. Furthermore, any part of the system that must carry or circulate borated water would need to be heated in order to ensure no boron crystallises which would limit the availability of boron in primary circuit and/or could form a blockage. This not only adds to the complexity of the plant as all circuits that carry boron must include adequate redundancy for heating and monitoring to ensure boron precipitation is avoided, but there is the added cost of operating and maintaining these systems. Only by total elimination of soluble boron could these drawbacks be completely avoided.

Once boron is injected into the primary circuit, a system must be in place to remove this boron for
the reactor to restart. The presence of this system adds further to maintenance and capital costs. It may be possible to avoid the need for this system by assuming that once the emergency boron system is activated the ship must return to port using a small auxiliary power system and the port would include the facilities that can remove boron from the primary circuit.

It has been stated, and is usually considered to be the case, that soluble boron acts as a diverse means of control from control rods in conventional PWRs [92]. However, in conventional PWRs, there are periods in time where the rod worth of all of the rods is not sufficient to achieve an acceptable shutdown margin if the SB were to be completely removed. Hence, SB and control rods are not truly redundant and diverse [91, 96]. Therefore, the loss of ‘diversity’ by removing chemical shutdown control is not as great as is often implied.

2.7 Fuel Elements

2.7.1 Fuel

Virtually all commercial power plants operating to date use uranium dioxide (UO$_2$) fuel. A notable exception is the Magnox reactors operating in the UK. In the early days of nuclear development a variety of fuels were investigated including uranium metals. Pure uranium is advantageous from a nuclear physics perspective as it has a very high theoretical density (19.1 g/cm$^3$) and therefore the highest ‘uranium density’, i.e. the mass of uranium per unit volume; this means that, for a given core volume, a reactor can contain more fissile material and therefore requires lower enrichment. Furthermore, the fact that uranium metal consists of effectively pure uranium, plus some minor trace impurities (<0.1%) that are still present after extraction, implies that there are fewer undesired atoms that can absorb neutrons. However, pure uranium metal suffers from two very significant disadvantages. Firstly, although the fuel is always contained in a cladding material that is compatible with both the coolant and the fuel, uranium metal is highly reactive with many coolants and is not suitable for use with high pressure water. Secondly, uranium metal’s complex crystal structure leads to poor thermal cycling and irradiation properties [58, 63].

Due to uranium metal’s high U density, it found applications in the early days of nuclear development, in reactors used for the producing of weapons-grade plutonium where enrichment had limited availability. This explains the interest in the UK for graphite-moderated reactors fuelled with U metal fuel [58]. Whilst uranium metals have been used in thermal reactors, they place very strict
limitations on temperature and burnup [63]. For these reasons a replacement to uranium metal was investigated. A material with low coolant chemical reactivity, good high temperature stability and a crystal structure which is more robust against irradiation damage and thermal cycling issues was thus sought. Finally, since the material was to be deployed on a large scale, it had to be readily manufacturable. The first two of these requisites are commonly associated with ceramics and all are satisfied by uranium dioxide. Consequently, for the development of a civilian reactor uranium dioxide was pursued [63].

There are some drawbacks relating to uranium dioxide, principally due to its brittle nature and very low thermal conductivity. These two properties imply that under modest thermal stresses cracking begins to develop. However, many of the issues related to cracking are readily solved by using an appropriate structural cladding. The low thermal conductivity is a more serious drawback, although it is offset by UO$_2$’s very high melting point (around 2800°C) and the fact that there are no phase changes right up to the melting point [58]. Furthermore, it has generally good irradiation behaviour and it also takes its chemically rather similar fissile and fertile relatives (plutonium dioxide and thorium dioxide) into solid solution across a large range of compositions [63].

Once it was discovered that UO$_2$ had many desirable properties a large scientific undertaking was initiated to use UO$_2$ in the Shippingport PWR demonstrator [63]. The successful demonstration of UO$_2$ fuel in the Shippingport reactor led to the use of this material in BWR and Pressurised Heavy Water Reactor demonstrators. Furthermore, UO$_2$ fuel was used in the successor to the Magnox reactors in the UK: Advanced Gas-cooled Reactors (AGRs)$^5$.

Other ceramics have been researched for use in reactors, namely uranium carbide (UC) and uranium nitride (UN). However, neither of these have been deployed on a commercial scale and research has mainly focused on their deployment in fast reactors. These ceramics have significantly higher thermal conductivity and higher uranium densities (both around 13 g/cm$^3$); however, they suffer from a number of drawbacks. In the case of UC, its chemical reactivity is problematic in the sense that its pyrophoric nature complicates manufacturing and it readily reacts with water, with the latter effectively precluding its use with this coolant [58]. Also, UC swells significantly more than UO$_2$ fuel and this can lead to clad degradation [62]. UN is also chemically reactive with both air and water but much less so than UC. A more significant drawback with regards to UN are issues relating to $^{14}$N,

$^5$AGRs adopted UO$_2$ fuel principally because their design required fuel capable of operating at temperatures beyond those permitted in Magnox fuel and UO$_2$ had been successfully demonstrated in a number of reactor types [58].
which constitutes around 99.5% of naturally occurring nitrogen; this nuclide has a moderately high absorption cross-section, which not only reduces the benefits of its high uranium density but leads to the production of $^{14}$C, complicating both reprocessing and geological disposal. These problems could be overcome by nitrogen enrichment, although the economics surrounding this are uncertain [62].

There are a number of other fuel types including metallic dispersion fuels and ceramic-metallic (cermet) fuels that can and have been used in PWRs [58, 62] (see Section 1.2.3 in the previous chapter). However, their very low uranium densities imply significant enrichment penalties, and for a long-life core like the one being studied here would likely necessitate enrichment above 20 wt.%. Therefore, given UO$_2$’s large scale successful deployment and the drawbacks of the other potential fuels discussed it has been judged that using UO$_2$ is a requirement for this reactor system, in order for the final design to be classified as using conventional LWR technology.

### 2.7.2 Fuel Element Geometry

To date, cylindrical rods have been the predominant fuel element geometry used in light water reactors. Plate fuel containing UO$_2$ has been used in some cores, for example in one of the core loadings in Shippingport [103] and in research reactors using so-called ‘Caramel’ fuel. In addition, a variant of Caramel fuel is used in French submarines [104]. However, UO$_2$ fuel poses some significant difficulties when used in the form of plates. Firstly, for a given thickness, a rod geometry will have a lower centreline temperature than that of a wide UO$_2$ plate, simply because the rod geometry will have a greater surface area in contact with coolant. To get around this issue the plate fuel based on UO$_2$ that has been used in some research reactors uses thin (1.45 mm thick) platelets, called Caramels, which have dimensions of around 17 mm by 17 mm. Each platelet is separated from its neighbouring platelet by 1.45 mm, with the space occupied by Zircaloy separators and clad in 0.4 mm thick Zircaloy; see Figure 2.1. This to some extent mimics so-called ceramic-metallic (cermet) fuel by combining UO$_2$ within an inert metal matrix, which in this case is Zircaloy $^6$. In comparison to conventional UO$_2$ fuel rods, the mass of zirconium to uranium in this Caramel design is relatively high, which will inevitably create an enrichment penalty due to the parasitic absorption of neutrons by zirconium. In addition, by reducing the mass of available fuel within the fuel element, there will inevitably be an increase in the burnup for a given power history. This latter point is a particularly strong drawback because

$^6$Cermet fuels typically utilise small spherical nuclear fuel particles within a matrix, rather than relatively large nuclear fuel platelets.
whilst the plate fuel will run cooler by being very thin and surrounded by a conductive metal matrix, it has limited free space to accommodate fission gas release and swelling. At burnups greater than approximately 60 GW.d/tHM the clad fails as the clad that is bonded to the Zircaloy separators is no longer able to withstand the internal fission gas pressure [27]. By comparison, cylindrical rods containing UO$_2$ have been shown to withstand burnups in excess of 95 GW.d/tHM [39].

![Diagram of plate fuel](image)

Figure 2.1: Caramel fuel plate (not to scale) [27].

One very significant advantage of plate fuel is the higher surface area to volume ratio compared to a conventional rod geometry. This implies that the heat flux will be much lower and therefore peak clad temperatures will be reduced. In principle, rod geometry could have a larger surface area to volume ratio by making the rods sufficiently small. However, in reality this is not possible due to the lack of rigidity in very thin, long metal tubes. This is much less of a problem for thin plates as their geometry imparts a far greater degree of rigidity and therefore they are more practical as an element for core construction.

There are practical issues regarding the use of plate fuel which were discussed above, namely regarding the fact that it appears unwise to adopt a fuel form that contains a large ratio of a non-fissile metal to uranium, and/or has rather tight limits on burnup tolerance. It would be possible to construct a core containing such fuel if a large number of plates were adopted, thereby increasing the mass of available fuel, ensuring enrichment is below the HEU limit and reducing burnup, but this would increase the size core relative to a UO$_2$ core. Furthermore, the publicly available information on their fuel performance under normal LWR conditions is minimal in comparison to cylindrical UO$_2$
rods. For these reasons it was decided to put in place the requirement that the core design must use cylindrical rods.

Related to rod geometry is the lattice geometry the reactor employs, and therefore the shape of the fuel assemblies. Fundamentally, lattices can either be triangular or rectangular, and typically the resulting assembly geometries are hexagonal or square. Given that a long core life was targeted it would have been prudent for the first iteration of the core design to employ a lattice geometry that maximises the number of rods inserted into the core. Hence, a preference for hexagonal assemblies emerges. However, a limitation developed due to the fact that the deterministic versions of the reactor physics software available for use in this investigation, for determining the behaviour of finite cores, is only able to model cores constructed of square assemblies.

The final limitation relating to core design was that the reactor should consist of rods with identical dimensions (i.e. the same pellet geometry and a fixed pellet-clad gap for all fuel rods throughout the core), this reduces manufacturing costs but was also to lessen the number of variables.

### 2.7.3 Cladding

Currently only two material types have been used to a large extent as cladding in LWRs; these are stainless steel, in particular type 304, and zirconium-based alloys. Stainless Steel (SS) was used extensively in demonstrator and commercial prototypes. Stainless steel displayed generally very good performance in earlier generation PWRs, however its behaviour in BWRs was poor, with failure rates of around 10% as burnup reached 17 GW.d/tHM [105]. Therefore, attention turned to developing zirconium-based clad for BWRs and this resulted in failure rates in BWRs dropping dramatically to less than 0.03% at average burnups of 17 GW.d/tHM [105]; these have since fallen much further. The satisfactory demonstration of Zr alloys in BWRs and the significantly lower thermal neutron capture cross-section of these alloys in comparison to stainless steels led to the replacement of SS in PWRs with Zr [105]. The earlier generation stainless steels also showed no net benefit in terms of corrosion performance at normal operation temperatures and comparably high oxidation kinetics at clad temperatures above 1200°C. In addition, all variants of SS suffer from enhanced tritium release. Zr alloys typically release less than 1% of the tritium produced in the fuel, whereas tritium readily escapes through SS, resulting in the reduction of a significant benefit of operating the reactor without SB [99] (see Section 2.6.3). Advanced SS alloys have been proposed for future LWRs and could result in characteristics favourable in certain accident conditions and/or reduced oxidation kinetics.
at normal operation temperatures; however, currently these benefits are not sufficiently developed to permit them to be used in LWRs [99]. Hence, only zirconium-based alloys will be considered for the reactor being designed in this study. However, it would not be possible to use conventional zirconium alloys and expose them to the temperatures normally found in large reactors for a 15 year period, simply because the cladding would not survive for such an extended period of time. No data was found on the corrosion performance of conventional PWR cladding materials exposed to typical in-reactor conditions, i.e. appropriate thermal gradients, neutron irradiation, chemical environment and coolant temperatures, for periods comparable to the targeted core life of 15 years. However, CANDU reactors, a type of Pressurised Heavy Water Reactor (PHWR), contain core components constructed from zirconium alloys that reside within the core for periods of time measured in decades [106].

CANDU reactors are unique in a number of ways. Firstly, their use of heavy water permits them to avoid the use of enriched uranium, although at the considerable expense of using large quantities of isotopically enriched heavy water. Heavy water possesses a very low thermal neutron absorption cross-section in comparison to light water (macroscopic epithermal absorption cross-sections are $2.3 \, \text{m}^{-1}$ and $3.7 \times 10^{-3} \, \text{m}^{-1}$ respectively). However, its macroscopic scattering cross-section and its average logarithmic energy decrement per collision are much smaller than light water, $154 \, \text{m}^{-1}$ vs $35 \, \text{m}^{-1}$, and 0.927 vs 0.510, respectively. This implies that a much larger volume of moderator is necessary to ensure sufficient collisions to take neutrons from their high energies at birth, to the lower thermal energies required to initiate a fission reaction with a high probability [107]. These characteristics require the active core length to be large (around 6 m vs 3.65 m for a conventional PWR), and by utilising unenriched fuel their average fuel discharge burnup is low in comparison to enriched LWR fuel (typically around 7 GW.d/tHM compared to around 50 GW.d/tHM) [58]. The CANDU system is also refuelled on power, and this process is made easier by arranging the tubes that contain the fuel assemblies horizontally. The fuel assemblies are also very short (around 50 cm) in order to achieve a higher mean-burnup before they are ejected and they typically reside within the core for around 300 days, with the clad surrounding the UO$_2$ pellets being Zircaloy-2 [108].

The horizontal tubes that contain the fuel assemblies are referred to as Pressure Tubes (PTs) and they function as mini pressure vessels in a CANDU system. It is these tubes that are of interest as a proxy for fuel clad as they reside within the core for around 10 years or more, and are constructed of zirconium-based alloys. The PTs have lengths of around 6 m, with an inner diameter of 103 mm and a wall thickness of 4.2 mm (which is around a factor of ten thicker than the clad in PWR fuel) [106].
The horizontal tubes penetrate a large low-pressure tank of heavy water that is kept at temperatures below 60°C. A typical CANDU system has 380 such pressure tubes. Figure 2.2 shows the layout of a CANDU system.


Due to the unenriched nature of CANDU fuel and its on power refuelling, there is no requirement for soluble boron. The pH of the primary coolant is currently kept in the region of 10-10.2 [106]. It is therefore expected that the pressure tube chemical conditions will be similar to those in the reactor being designed in this study, as there is a preference for no SB in the marine core and there is no boric acid in the primary coolant of CANDU systems.

If a zirconium-based alloy is used in the reactor being studied in this work, then the coolant temperature will need to decrease significantly from that in a conventional LWR in order to limit degradation from corrosion related phenomena. Originally CANDU systems operated at much lower temperatures than the current CANDU 6 systems, although the geometry and burnup were similar to current CANDU systems. Data on earlier CANDU systems, that operated at lower temperatures, was thus collated and corrosion performance is summarised in Figure 2.3.
Figure 2.3 clearly shows the significantly improved oxidation performance as outlet temperature is reduced, along with the dependence on Zr alloy type. Figure 2.3 also includes the usual oxidation limit imposed on the clad, which for a typical 0.572 mm clad wall thickness is 57.2 μm.

Besides oxidation, the uptake of hydrogen is also an important clad degradation mechanism. Zirconium has a very high affinity for hydrogen but also a very low solubility limit for the substance, which decreases dramatically as a function of temperature; for instance at 300 °C the solubility limit is 80 wt. ppm compared to 200 wt. ppm at 400 °C [109]. Once the solubility limit has been reached, the hydrogen precipitates out of the solid solution as a zirconium hydride phase (ZrH$_{1.6}$ or ZrH$_2$). Zirconium hydride has the characteristic of being very brittle and so can embrittle the clad, thereby reducing its fracture toughness and increasing its susceptibility to cracking. This is one advantage of stainless steel’s low affinity for hydrogen, although the downside, as discussed earlier, is the much higher tritium release from the fuel rod.

The predominant source of the hydrogen absorbed by the clad is from the liberated hydrogen produced during oxidation [109]. Thus, by reducing the extent of oxidation occurring one reduces the extent of hydrogen absorption [30]. However, this will have little impact on other potential sources of hydrogen, such as (n,p) reactions with the clad material and hydrogen produced by radiolysis of the coolant. As the oxidation rate decreases with lower temperatures, the terminal solubility limit also decreases. As other potential sources of hydrogen will still exist there may be some concern about operating the reactor at lower temperatures and the susceptibility of the clad to hydriding phenomena. Yet the available data on zirconium alloys at lower temperatures showed peaks in hydrogen
concentration positively correlated with higher neutron fluxes and oxide thicknesses, i.e. in general near the top of the core where the coolant temperature is higher [29]. Figure 2.4 shows the maximum hydrogen pickup for pressure tubes in low temperature CANDU systems, which also demonstrates improved hydriding performance at lower temperatures.

Pressure tubes are not exposed to identical PWR fuel cladding conditions. The main differences are that the neutron flux they are exposed to is an order of magnitude lower and the temperature gradient is also smaller, both of which significantly impact corrosion performance. However, PTs are exposed to temperatures in excess of 250°C [29]. CANDU PTs have used Zircaloy-2 in the past, a 1st generation Zr alloy also used as fuel cladding, but this has been superseded by alloy Zr-2.5Nb. Zircaloy-2 was used as the PT material when they resided within the core for periods of 10 years and coolant outlet temperatures were below 290°C. Its replacement, alloy Zr-2.5Nb, has shown superior corrosion performance and PTs of this material currently reside in CANDU reactors for periods up to 30 years with outlet temperatures increased to 313°C [106]. However, Zr-2.5Nb is inappropriate for use as a fuel cladding material due to its degraded mechanical performance, for instance its relative creep response is much higher (by around a factor of four) than Zircaloy-4 and ZIRLO [30]. This raises concerns that the clad would be more likely to fail given the similar ductile behaviour between the two alloys. Whilst alloy Zr-2.5Nb is not appropriate for fuel cladding in PWRs, its corrosion performance is expected to mimic 2nd generation PWR cladding materials such as ZIRLO to some extent. These second generation alloys have incorporated significant quantities of niobium and further adjusted other constituents of the alloy to significantly increase corrosion performance and therefore

Figure 2.4: In-reactor hydriding performance of Zircaloy-2 and Zr-2.5Nb pressure tubes at two distinct temperatures and fluxes (reproduced from data in [29] along with lines of best fit).
it was assumed that they would exhibit similar corrosion performance to Zr-2.5Nb. In order to test this hypothesis published data on their performance was compared to Zr-2.5Nb. Figures 2.5 and 2.6 summarise their relative corrosion performance.

As lithium hydroxide is used to control the pH in CANDU and PWR systems, it is important to compare the performance of the zirconium-based alloys in the presence of typical (of the order of 1 ppm) lithium concentrations. At lithium concentrations of 3.5 ppm over an exposure period of 112 days, there were no discernible impact on corrosion performance between the Zr-2.5Nb, ZIRLO and Zircaloy-4 [30].

Furthermore, the advanced zirconium alloys assumed to be deployed in this core design are far more
resistant to hydriding than earlier generations of Zircaloy. For instance, the hydrogen pickup rates at a temperature of 316 °C after exposure for 852 days were 0.6 µg/dm²/day for ZIRLO, 0.5 µg/dm²/day for Zr-2.5Nb and 3.4 µg/dm²/day for Zircaloy-4 [30]. Therefore, it appears to be the case that the hydriding and oxidation performance of ZIRLO and Zr-2.5Nb are similar at low temperatures (less than approximately 310°C).

Unsurprisingly, given the data summarised above, there are significant margins, with respect to oxidation and hydriding performance, for increasing the primary coolant temperature in CANDU systems and this has indeed occurred. Inlet temperatures and outlet temperatures have risen by around 15°C and the flux has also increased by roughly a factor of 2. Zr-2.5Nb has operated successfully in CANDU systems at these higher temperature up to 20 Effective Full Power Years (EFPYs) and PTs have been developed to operate up to 30 EFPYs for the currently in-service CANDU systems. However, due to the uncertainty surrounding the assumption that Zr-2.5Nb and 2nd generation zirconium-based alloys, such as ZIRLO, exhibit comparable corrosion performance at temperatures less than approximately 310°C in high pH water, and the fact that CANDU PTs can only be used as a proxy for PWR fuel clad, the coolant outlet temperature has been restricted to < 290°C, with peak clad temperatures less than approximately 310°C. The latter temperature limit is simply based on the outlet temperature on more recent CANDU systems, which is 313°C. For comparison, current large light water reactors have inlet and outlet temperatures of around 290°C and 320°C respectively and peak clad temperatures around 350°C. The temperature rise across the reactor being designed in this study is unknown given that this would require a full analysis of the primary and secondary circuit, which is beyond the scope of this investigation. Therefore it is assumed that the temperature rise in the marine reactor will be approximately the same as in large light water reactors, i.e. around 30°C.

As early CANDU PT designs have been used as a guide for corrosion characteristics it was decided that the coolant mean temperature of the system being designed should be the same as the mean coolant temperature in these early CANDU systems, which was 270°C. This is because mean coolant temperatures more accurately correlate with where the harshest material conditions are in the core than outlet temperatures alone. This is due to the detrimental impacts of neutron and gamma fluxes, both of which tend to peak in the centre of nuclear reactor cores. In addition, the heat flux, which is correlated also with the highest pin powers, tends to peak in the central region of the core. Hence, it seemed appropriate to weight the coolant temperature to these adverse effects. Therefore given a
30°C rise, this implies an inlet temperature of 255°C and outlet temperature of 285°C.

Given the low coolant outlet temperatures needed to ensure the survivability of the clad over such long time periods, this will ultimately determine the thermal efficiency of the marine nuclear power plant. Conventional reactors have quite complex secondary circuits in order to extract as much electrical power from the plant as is possible. This involves reheating steam outlets and bypassing outlets to different turbines. It is unlikely such a complex secondary circuit would be viable due to the low temperature of the outlet in the reactor being designed in this study or that it would even be warranted if the aim is to reduce the plant’s complexity for a small team to operate and maintain. It was therefore assumed that plant efficiency would be around 25% (for comparison a conventional reactor has a thermal efficiency of around 32%). Hence, given the plant is required to produce 110 MWe and thermal efficiency is assumed to be 25%, the thermal output is 440 MWth. Factoring in a Capacity Factor (CF) of 93.5% results in an average thermal power of 411.4 MWth. A requirement is now given for the average thermal power output the core must provide over its 15 year core life.

Finally, it is worth mentioning that normally reactor designers avoid lowering the inlet temperatures considerably outside of existing operating experience due to the uncertainty this may cause in relation to RPV embrittlement, as it is expected that thermal annealing will be reduced and RPV fracture may arise at some point in time. However, this is unlikely to be prohibitive for this reactor concept for a number of reasons. Firstly, the RPV life is considerably lower than conventional reactors (30 years vs 60 years). Secondly, the lower power density of the fuel implies that the total fluence the RPV will experience will be considerably lower than typical RPV exposures. Finally, if there were concerns regarding embrittlement over the life of the reactor, then it is possible to envisage mid-life annealing of the RPV taking place in-situ. This could consist of electrically heated elements surrounding the RPV being employed during one of its refuelling outages.

### 2.8 Burnable Poisons

Burnable Poisons (BPs) provide an important way of controlling the reactivity in a core. At the start of life the fuel is at its most reactive and without any reactivity control this core would simply decline in reactivity with burnup. Control rods can be used to manage excess reactivity by placing them deeply into the core early in life but this is a relatively coarse form of control and has many other
disadvantages. For example, there can be large nonuniform distribution in axial neutron flux profile; instead BPs are relied more heavily upon to provide a finer degree of reactivity control. In addition, BPs can be used to alter the power profile of the core and therefore limit to some extent the size of local peaking factors across the core.

There are many potential neutron absorbers that could be used as burnable poisons. The elements that behave as burnable poisons are: silver (Ag), gold (Au), boron (B), cadmium (Cd), dysprosium (Dy), erbium (Er), europium (Eu), gadolinium (Gd), hafnium (Hf), mercury (Hg), holmium (Ho), indium (In), iridium (Ir), lutetium (Lu), rhenium (Re), rhodium (Rh), samarium (Sm), tantalum (Ta) and thulium (Tm) [110]. However, realistically only a few of these would be appropriate, as many would have a very high residual poison penalty, some are very weak absorbers (lutetium and tantalum), some are very rare and others have not been used in reactors and would require extensive irradiation testing and material property characterisation to be performed.

Boron was ruled out as a heterogeneous (solid) poison for the reactor being studied here, even though it is used in some PWRs as a BP. Given the long core life targeted, and therefore the likely need for large concentrations of solid BPs to control excess reactivity, this would result in considerably higher quantities of boron required than has ever been experimented with in conventional fuel rods. If boron was utilised then this would very likely lead to excessive amount of helium (He) being produced and therefore considerably raise the rod internal pressure without a very large plenum volume present. Consequently, the remaining poisons listed - gadolinium, hafnium, europium, erbium and dysprosium - were considered in more detail. Table 2.1 lists some important neutronic properties of these poisons.

<table>
<thead>
<tr>
<th></th>
<th>Gd</th>
<th>Eu</th>
<th>Dy</th>
<th>Er</th>
<th>Hf</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal cross-section (barns)</td>
<td>4900</td>
<td>4600</td>
<td>930</td>
<td>162</td>
<td>105</td>
</tr>
<tr>
<td>Resonance integral (barns)</td>
<td>390</td>
<td>2430</td>
<td>1600</td>
<td>740</td>
<td>1980</td>
</tr>
<tr>
<td>Resonance range</td>
<td>1.1 - 1300 eV</td>
<td>1.1 - 150 eV</td>
<td>1.1 - 150 eV</td>
<td>0.1 - 56 eV</td>
<td>1.0 - 200 eV</td>
</tr>
</tbody>
</table>

Table 2.1: Neutronic properties of some key burnable poisons [9, 10, 11]. Note that gadolinium is distinct from the other burnable poisons represented here as it consists of only two highly absorbing isotopes, $^{155}\text{Gd}$ and $^{157}\text{Gd}$, whose thermal absorption cross-sections are extremely high, $61 \times 10^3$ b and $254 \times 10^3$ b respectively. Together these two isotopes have an abundance of around 30% in natural gadolinium (gadolinium’s remaining isotopes are effectively transparent to neutrons).
Of the elements listed in Table 2.1 gadolinium and erbium have been used widely in PWRs with gadolinium now the most commonly used burnable poison in PWRs [111]. It is to be noted that hafnium, europium and dysprosium have the longest isotope chains in which several isotopes participate in the absorption phenomenon (see Table 2.2 in Section 2.9 regarding the abundance of certain nuclides in materials used for control rods). Hafnium and europium also generate some very absorbent non-natural isotopes by neutron capture, and in the case of europium, transmute into nuclides that are also very absorbing (for example Eu can beta-decay to $^{155}$Gd and $^{157}$Gd). This behaviour means that residual poisoning can be high [11, 112]. However, these elements could in principle be mixed with low residual poison elements, such as gadolinium, in order to slow the depletion of one poison relative to the other.

It should be noted that besides the neutronic properties of burnable poisons that are incorporated into fuel rods, it is also important to consider how the poison impacts the material characteristics of the nuclear fuel. For example, the poison’s impact on thermal conductivity, irradiation behaviour, chemical compatibility with the constituents of the fuel rod and how it impacts the sintering procedure carried out in the production of ceramic pellets. Therefore, as there is little available data on such material characteristics for hybrid poisons, it makes it difficult to consider how hybrid poisons could be realistically deployed in a commercial fuel rod. This highlights an area for potential future work.

Another strategy would be to increase the concentration of gadolinium isotopes with large thermal neutron absorption cross-sections relative to the weaker neutron absorber isotopes. This strategy would be acceptable but is not commercially developed and therefore the economics are uncertain. Therefore it was decided to focus on unenriched Gd and Er.

### 2.9 Control Rods

Table 2.2 shows key nuclides deployed in various control rod materials.

Conventional PWRs use Rod Control Cluster Assemblies (RCCAs) which, in the case of 17 by 17 assemblies, consist of 24 rods of a neutron-absorbing material. The predominant absorbing material in use has been a metallic alloy consisting of 80% silver, 15% indium and 5% cadmium (Ag-In-Cd) [113]. As stated in the Section 2.6, PWRs normally use soluble boron to control reactivity and therefore control rods have typically been used for core shutdown, rather than for compensating the long-term reactivity changes associated with depletion of fuel, depletion of burnable absorber and fission product.
Nuclide | Isotopic abundance | Thermal absorption cross-section (barns)
---|---|---
$^{10}$B | 0.199 | 3800
$^{107}$Ag | 0.518 | 31
$^{109}$Ag | 0.482 | 87
$^{113}$Cd | 0.122 | 20000
$^{113}$In | 0.043 | 58
$^{115}$In | 0.957 | 210
$^{174}$Hf | 0.0016 | 1500
$^{176}$Hf | 0.0521 | 15
$^{177}$Hf | 0.1861 | 380
$^{178}$Hf | 0.2730 | 75
$^{179}$Hf | 0.1363 | 65
$^{180}$Hf | 0.3563 | 14
$^{160}$Dy | 0.023 | 130
$^{161}$Dy | 0.189 | 680
$^{162}$Dy | 0.255 | 240
$^{163}$Dy | 0.250 | 220
$^{164}$Dy | 0.282 | 2780

Table 2.2: Thermal absorption cross-section and isotopic abundance for key nuclides used in control rods.

<table>
<thead>
<tr>
<th>Material</th>
<th>Thermal absorption macroscopic cross-section (cm$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>B$_4$C</td>
<td>81</td>
</tr>
<tr>
<td>Ag-In-Cd</td>
<td>9.9</td>
</tr>
<tr>
<td>Hf</td>
<td>4.8</td>
</tr>
<tr>
<td>HfB$_2$</td>
<td>55</td>
</tr>
<tr>
<td>Dy$_2$HfO$_5$</td>
<td>13</td>
</tr>
<tr>
<td>Dy$_2$TiO$_5$</td>
<td>18</td>
</tr>
</tbody>
</table>

Table 2.3: Thermal absorption macroscopic cross-sections of materials that have been researched for use in control rods [12, 13, 14].

buildup. BWRs on the other hand do not use soluble boron and their control rods - in the form of blades - are constantly penetrating a significant proportion of the active fuel region. All BWRs use cruciform shaped control rod blades (CRBs) that fit in between the fuel assemblies. The CRBs have four wings, with each wing containing absorber rods that are normally filled with boron carbide powder [113].

Both Ag-In-Cd and B$_4$C undergo swelling during irradiation; in the former this is due to the conversion of In into Sn, and Ag into Cd, whereas irradiated $^{10}$B leads to the formation of lithium and helium [113]. Swelling is less of a concern in PWR rods, in part because swelling is lower in Ag-In-Cd but also because they typically experience much lower neutron fluences [114]. Ag-In-Cd suffers
from a number of other weaknesses, one being its low melting point which results in it being the first material in a reactor to undergo melting in severe LOCAs [12]. Also the relative expense of Ag-In-Cd in comparison to other potential absorbers such as boron carbide and lower absorption cross-section make it unfavourable for deployment in the reactor being designed in this study (see Tables 2.1 and 2.2). B$_4$C also has the benefits of high adjustable efficiency through enrichment (i.e. by increasing the concentration of $^{10}$B relative to $^{11}$B), lower mass (which is important when considering the mechanical design limits of Control Rod Drive Mechanisms (CRDMs)) and the fact that it creates low radioactive waste streams due to benign transmutation products. Furthermore, it is not believed that any reactor type has ever used Ag-In-Cd control rods in a manner comparable to how they will be required to function in a Soluble Boron Free (SBF) designed core, i.e. large proportions of the rods penetrating in the core for very long time periods. This is probably due to the neutronic characteristics of Ag-In-Cd, where $^{113}$Cd is the strongest thermal absorber but accounts for only a small proportion of the available nuclides within the Ag-In-Cd alloy. Therefore, it is to be expected that this single isotope will burn out relatively quickly, greatly diminishing the rod worth [12]. For these reasons Ag-In-Cd will not be considered as a control rod material for the reactor being studied in this investigation.

Until fairly recently the absorbing materials in LWRs consisted of one of the two neutron poisons Ag-In-Cd and B$_4$C, with some PWR vendors having used a hybrid control rod design that consisted of Ag-In-Cd in the lower portion of the control rod and the remainder containing B$_4$C [115]. Utilising two distinct materials permits a degree of optimisation by benefiting from Ag-In-Cd’s lower swelling rates in comparison with B$_4$C but reducing detriments associated with higher costs and weaker absorption relative to B$_4$C [114]. This hybrid method has also recently been adopted in BWRs. However, BWRs have utilised hafnium in the lower portion of the control blades. These hybrid Hf/B$_4$C blades are currently being introduced into BWRs as older CRB designs are coming to the end of their designed lifetime [113].

It is worth noting that whilst in principle boron carbide does have a much higher melting temperature than Ag-In-Cd (2470°C vs 800°C), the fact that it may undergo a eutectic reaction with stainless steel, and other materials usually used in nuclear reactors, such as Inconel, reduces its effective melting point considerably. This eutectic reaction commences at 1030°C, although rapid liquidification does not take place until around 1280°C [115]. Yet this is still significantly higher than Ag-In-Cd’s melting point. Hafnium on the other hand undergoes melting at 2150°C and does not have a eutectic reaction with stainless steel or zirconium-based materials [115]. Although severe accidents may result in core
temperatures above approximately 1200°C, which is the temperature limit where extensive oxidation of Hf with high temperature steam can take place, as is the case with zirconium-based alloys and boron carbide [116, 117]. This is clearly a drawback of utilising Hf and B$_4$C compared to Ag-In-Cd, but given that B$_4$C and Hf are used in licensable reactor designs this is clearly not prohibitive.

Other absorber materials that have received attention, to varying extents, for use in control rods include hafnium diboride (HfB$_2$), dysprosium titanate and dysprosium hafnate [12, 14, 118]. However, apart from some recent Russian experience in PWRs with dysprosium titanate, these materials are not as well developed as Ag-In-Cd, B$_4$C or Hf. Therefore, given that Hf has been used in PWRs and also more recently in BWRs under similar conditions as are intended in this work, i.e. high penetration into the active core region during burnup for long periods of time, it is the prime candidate for use in this reactor system as a replacement for Ag-In-Cd. And therefore Hf rods or Hf/B$_4$C hybrid rod designs can be considered as conventional LWR technology.

2.10 Parameters Summary

The aim of this section was to determine the requirements, goals and limitations with respect to key parameters necessary for design work to begin. The requirements are:

- $^{235}$U enrichment must be below 20 wt. %. 
- Conventional LWR technology must be employed. This has been determined as using cylindrical fuel rods containing UO$_2$ fuel pellets clad in a zirconium-based alloy, with either erbium or unenriched gadolinium oxide used as the burnable poison. In addition, control rods based on hafnium and/or boron carbide must be used.
- In order to have some confidence in the ability of the zirconium-based clad to survive for the targeted core life of 15 years, the inlet temperature has been set to 255°C and an outlet temperature of 285°C, with peak clad surface temperature less than 310°C.
- The core must produce 411.4 MWth, based on a maximum output of 110 MWe, with a capacity factor of 93.5% and assuming a thermal efficiency of 25%.

The following goals have been put in place:
• A preference for soluble-boron-free operation. For this to be considered a viable strategy, ejection of any single RCCA must not result in prompt criticality. Also, the core must ensure satisfactory shutdown margins from hot full power to cold zero power with no xenon present conditions.

• Core life of 15 years targeted.

• Fuel assemblies should fit inside a 3.5 m outer diameter reactor pressure vessel.

Finally, the following limitations are in place:

• Square assemblies.

• All fuel rods have the same dimensions.
Chapter 3

Uranium Core

3.1 Outline

A number of small modular reactor core designs that aim to achieve long-lives (> 5 years) utilising conventional light water reactor technology are listed in Ref. [119]. However, there appears to be very limited (if any) published 3D core analysis of either neutronic behaviour or fuel performance for these reactor systems. There has been some detailed neutronic analysis looking at extending the fuel cycles in large (~1 GW(e)) PWR systems up to around 3 years [120] and studies assessing the neutronic characteristics of a large PWR system operating without soluble boron with fuel cycles less than 3 years [121, 122]. By constructing a core model based on the parameters defined in the previous chapter, which are summarised in Table 3.1, a core has been designed specifically for powering a large civilian container ship. In addition, gaps in the available literature regarding long-life soluble boron free PWR systems are addressed.

Further refinements were made to the core parameters in this chapter, in particular selecting either gadolinia or erbia as the burnable poison and the fuel rod dimensions. Then a core loading pattern was created and the constructed core model was assessed in terms of its neutronic and fuel performance behaviour.

Key neutronic characteristics that the core was investigated against include:

- The shutdown (sub-criticality) margin once all control rods are inserted into the core;

- Core behaviour caused by potential faults that can lead to the removal of a number of control
Table 3.1: Summary of key parameters for the reactor being designed in this study.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal Output</td>
<td>440 MWth</td>
</tr>
<tr>
<td>Thermal Efficiency</td>
<td>25%</td>
</tr>
<tr>
<td>Capacity Factor</td>
<td>93.5%</td>
</tr>
<tr>
<td>Fuel</td>
<td>UO₂</td>
</tr>
<tr>
<td>Lattice Type</td>
<td>Square assembly</td>
</tr>
<tr>
<td>Cladding</td>
<td>2nd Generation Zr alloy (e.g. Zirlo)</td>
</tr>
<tr>
<td>RPV Outer Diameter</td>
<td>3.5 m</td>
</tr>
<tr>
<td>Targeted Core Life</td>
<td>15 years</td>
</tr>
<tr>
<td>Average Coolant Temperature</td>
<td>270°C</td>
</tr>
</tbody>
</table>

- Reactivity coefficients, which are used to determine the core’s response to changes in power output;
- Power distribution within the core under normal operating conditions;
- The effects xenon can have on core reactivity and power distribution.

Key fuel performance criteria the core was investigated against include:

- The likelihood of clad rupture caused by excessively high rod internal pressure due to fission gases and pellet swelling;
- Pellet Clad Interaction (PCI), which is a failure mechanism that arises when a fuel rod experiences a rise in power. This rise in power can lead to the pellet imposing high amounts of stress on the clad and chemically aggressive fission products attacking the clad material.

### 3.2 Codes

When designing a reactor core it is typical to model the neutronics, fuel performance and thermal-hydraulics separately due to the inherent difficulty in trying to couple all three phenomena within one computer program. However, as all three calculations have some degree of mutual dependence, such as fuel rod geometry affecting: the pellet temperature; the fluid dynamics; and the reactivity of the fuel, it is necessary to update mutually dependent variables. Therefore as the core becomes more refined its overall behaviour can be determined with a high degree of accuracy.
In this study only the neutronics and fuel performance are analysed in detail as it is important to determine the necessary rod geometry before detailed thermal-hydraulics calculations can be performed. Hence, the following four codes have been utilised:

- **CASMO-4** - a multi-group two-dimensional neutron transport theory code for modelling fuel assemblies. This has been used extensively within the nuclear industry, in combination with SIMULATE-3, for designing and licensing light water reactors [123].

- **SIMULATE-3** - a 3D nodal code that utilises diffusion theory. SIMULATE employs the output from CASMO-4 to create a finite 3D core and is used for determining the spatial and time dependence of the neutron flux throughout core life [124].

- **MONK-9A** - a Monte Carlo package for modelling neutron transport. MONK is a commercial Monte Carlo code for simulating the behaviour of neutrons within a reactor system and also has the capability of modelling the depletion of nuclides as a function of power output. MONK has undergone extensive validation for a variety of uranium and plutonium systems based on the data from the International Criticality Safety Benchmark Evaluation Project [125].

- **ENIGMA-7.8** - a 1.5D fuel performance code that has been widely deployed within the UK for modelling the behaviour of fuel in both gas-cooled and water-cooled reactors [126, 20].

### 3.2.1 CASMO

CASMO is a lattice code that calculates the change in fuel composition as a function of burnup on an assembly scale. CASMO attempts to solve the neutron transport equation in its time independent form. The neutron transport equation is

$$\frac{1}{v} \frac{\partial \Phi}{\partial t} + \hat{\Omega} \cdot \nabla \Phi + \Sigma_t \Phi = \int \int \Sigma'_s \Phi' dE' d\hat{\Omega}' + s,$$

(3.1)

where $\hat{\Omega}$ is the unit direction vector, $v$ the neutron speed, $\Phi$ the angular flux, $\Sigma_t$ the total macroscopic cross-section, $\Sigma_s$ the macroscopic scattering cross-section and $s$ the source term.

Due to the strong dependence of material cross-sections as a function of neutron energy, and the fact that neutron energies range from $10^7$ eV to $10^{-3}$ eV, it is necessary to perform calculations in a series of groups. In CASMO-4 a multi-group scheme consisting of 70 energy groups is utilised. As the lattice can be discretised into a series of so-called pin cells, a pin cell being a region containing...
the fuel rod (pin) and its surrounding coolant, the calculation begins at this scale, within each of the
energy groups.

Firstly, the average cross-section within the energy groups must be determined by weighting the
neutron cross-section, \( \sigma(E) \), by the neutron flux within the energy group. However, as the neutron
flux is yet to be determined, an approximation of the neutron flux must be introduced which assumes
the flux has a standard PWR flux distribution \([127]\). Subsequently the flux variation within each pin
cell, for each energy group, is computed using the method of collision probabilities, which treats the
rods as a 1D line source in order to determine the radial flux distribution across the cell (see Ref.
\([15]\) for further details). The updated flux is then used to determine the cross-sections within each
pin cell, and due to the fact that the flux within each pin cell is dependent upon its neighbouring pin
cells, these individual cells must be coupled together, which is achieved via surface currents.

Finally, in order to calculate the flux distribution throughout the lattice, the steady-state neutron
transport equation in its discretised form is subsequently solved along tracks that traverse the problem
\([128]\).

3.2.2 SIMULATE

A core will consist of several unique lattices (assemblies). These lattices will have differing numbers of
fuel rods at certain enrichments and also rods containing different concentrations of burnable poison.
Each unique lattice within the core is run in CASMO, and then the user specifies in SIMULATE the
3D layout of the core based on the lattices executed in CASMO \([129]\).

As the flux within each assembly is dependent upon its neighbouring assemblies it is necessary
to couple the assemblies together using surface currents. In addition, due to the fact that the core
is relatively large (much larger than an individual fuel pin) and that in order to determine the axial
variation of the flux within the core each assembly must be divided into approximately 20 axial regions,
the fluxes calculated in CASMO are reduced to 2 groups (a fast group, defined as being above 4 eV,
and a thermal group) to limit execution times \([15]\).

The flux throughout the core is determined using a 2 group form of the diffusion equation. Once
the flux distribution is known, SIMULATE then determines the power distribution across the core.
3.2.3 MONK

MONK is a Monte Carlo package that simulates the stochastic behaviour of a finite number of neutrons. Monte Carlo codes more accurately represent the geometry and the nuclear data than deterministic codes (such as CASMO-SIMULATE) but at the disadvantage of the statistical uncertainty associated with such a method. The uncertainty can be reduced by running the Monte Carlo code with more neutron histories but with a corresponding increase in computational cost. Therefore, in the case of burnup runs for the reactor under investigation in this study, this can result in time penalties two to three orders of magnitude larger than a deterministic technique. Hence, to date, Monte Carlo codes are used primarily for benchmarking or for evaluating cores which contain complex geometries where no satisfactory deterministic method has yet been proven to accurately model such a reactor type [20].

MONK simulates the birth, migration and eventual fate of a finite number of neutrons. The process consists of randomly sampling a series of probability distributions to determine the energy a neutron begins life with, the direction of travel, the outcome of an interaction (fission, inelastic scattering, absorption, etc.). If the outcome is fission, then the number of neutrons released must be determined. Because a single event is unlikely to be representative of the whole system, a number of histories must be evaluated to accurately determine the reactor state [130].

3.2.4 ENIGMA

As with many fuel performance codes ENIGMA models the fuel rod as a series of axial zones, with each section of the fuel rod assumed to have no axial or circumferential dependence [126, 20]. This results in a radial 1D representation of each section of the fuel rod, greatly diminishing the computational cost associated with modelling the behaviour of the fuel. By analysing the fuel rod at several axial locations, and coupling these axial regions when calculating the temperature rise of the coolant and fission gas transport, this results in a so-called 1.5D (or quasi-2D) representation of the fuel rod.

In order to accurately determine the behaviour of a fuel rod, its temperature profile must first be computed, as many mechanisms within the fuel, such as expansion and fission gas transport, are strongly temperature dependent. To determine the temperature distribution the equation of thermal conduction must be solved in a series of radial slices throughout the rod geometry. The equation of thermal conduction is
$$\frac{\partial (\rho c T)}{\partial t} - \nabla \cdot \lambda \nabla T = q'''(r, t),$$ (3.2)

where $T$ is the local temperature, $\rho$ is the material density, $\lambda$ is the thermal conductivity, $c$ the specific heat capacity and $q'''$ is the volumetric power density. The volumetric power density is determined in SIMULATE and the properties $\lambda$ and $c$ are determined by ENIGMA using correlations derived from empirical datasets.

Equation 3.2 is solved in its 1D time-independent form. From this calculation various mechanical phenomena including pellet thermal expansion (which can result in pellet cracking if internal stresses are sufficiently high), swelling and creep are modelled. Since these mechanical phenomena can alter the pellet geometry and therefore affect the pellet-clad gap size (which in turn strongly impacts the temperature of the fuel) the thermal and mechanical calculations are coupled. This is achieved by solving the mechanical and thermal equations separately, and updating mutually dependent variables via an iterative method.

A variety of phenomena are simulated in ENIGMA besides purely thermo-mechanical ones. These include clad embrittlement and corrosion, stress corrosion cracking and micro-structural changes in the fuel [20].

3.3 Neutronic Characteristics

3.3.1 Refinement of Parameters

The previous chapter came to the conclusion that a number of constraints would be put in place; these were: reactor pressure vessel outer diameter must be less than 3.5 m; square assemblies must be utilised; cylindrical rod geometry and either erbium or gadolinia burnable poison to be employed.

A standard 17 by 17 PWR assembly was chosen as this avoided the uncertainties associated with implementing a new grid design, namely that a new assembly geometry must undergo many thousands of hours of testing before confidence can be gained in successful implementation [131]. Standard 17 by 17 assemblies have dimensions of 21.42 cm by 21.42 cm and can accommodate fuel pins up to diameters of 1.06 cm [132].

\[1\text{Ref. } [132\text{] considers fuel pins up to 1.06 cm in diameter on a 1.26 cm pitch lattice. This appears to be a sensible upper limit on the fuel rods in conventional lattices and grid components holding the rod in place are unlikely to be less than 2 mm.}\]
As the pressure vessel’s outer diameter should be less than 3.5 m, this placed limitations on the permitted number of fuel assemblies within the core. With 17 by 17 assemblies, it was determined that the maximum number of assemblies that could fit into such a Reactor Pressure Vessel (RPV) was 89 assemblies. The outer diameter of this array of assemblies was 245.14 cm, and assuming an RPV thickness of approximately 20 cm implies a gap between the outermost assembly and the inside of the pressure vessel of approximately 30 cm (350 cm > 245.14 cm + 30 cm × 2 + 20 cm × 2). The 89-assembly limit was also chosen after investigating other SMR designs which had RPV outer diameter limits of 3.5 m, with the Westinghouse SMR also using 89 17 by 17 assemblies [133]. The active length of the fuel rod was set to 245.14 cm, which was equal to the diameter of the core.

![Figure 3.1: Maximum achievable core life as a function of initial heavy metal inventory (where the term heavy metal is defined as all elements above actinium in the periodic table), based on a CASMO run containing UO₂ rods in a 17 by 17 lattice geometry with an enrichment of 10 wt.%. Note that cores based on pellets up to radii of 0.4997 cm, which is beyond the 0.4646 cm limit imposed by the grid design are included; these extra data points were added in order to demonstrate the diminishing benefit associated with larger pins.](image)

Given the limited core size and the long core life targeted it appeared sensible to find the maximum amount of fuel the core could contain. However, simply inserting the largest rod size that the assemblies can accommodate is not necessarily an economic strategy since larger pin sizes result in lower Moderator to Fuel (M/F) ratios which can detrimentally affect the neutron economy. This is illustrated in Figure 3.1 which shows the effect of increasing the rod size on achievable core life. The achievable core life was determined by calculating when $k_{\infty}$ equalled 1.0 in a CASMO run consisting of an infinite array of 17 by 17 lattices, which contained 264 fuel rods (with the remaining 25 rod spaces being designated water channels, see Figure 3.3 for an example of a 17 by 17 lattice). A range
of fuel rod sizes were considered, which contained pellets with radii between 0.385 cm and 0.4646 cm. The pellet-clad gap size and clad thickness were set to $8.2 \times 10^{-3}$ cm and 0.0572 cm respectively, as is typical for PWR rods [16]. The lower bound for pellet sizes was determined by considering published designs for thin pellets [16], whereas the upper limit was set to 1.06 cm as conventional PWR grids are unlikely to be able to accommodate rods sizes greater than that [132]. All rods in Figure 3.1 had an enrichment of 10 wt.%, as this was the initial guess for the approximate enrichment necessary to achieve the 15 year targeted core life, also note that the rods contained only UO$_2$ with a density equal to 95% of the theoretical density (a typical density for UO$_2$ fuel [134]) and no burnable poison was present.

Figure 3.1 shows that for very large pellets there are diminishing returns in achievable core life as the total fissile mass is increased. Therefore, it is inappropriate to load the core with very fat fuel rods from an economic standpoint, as the greater fuel loading is having a limited effect on extending the achievable core life. A fuel inventory of 30.2 tonnes was chosen and this corresponded to a pellet radius of 0.4267 cm. Therefore, all subsequent core design work utilised pellets of this size.

As erbia and gadolinia appeared to be promising burnable poisons for deployment in this reactor concept, it was decided to construct lattice models in order to assess their ability to limit reactivity swing over core life. Reactivity swing is defined here as the difference between the minimum and maximum $k_{\infty}$ values over the course of core life. This is an important parameter as the core must operate with $k_{\text{eff}}$ equal to 1.0 during power operation. If the reactivity swing is large even with the addition of burnable poisons then this implies that the control rods (or soluble poison if present) must then ensure critical conditions. Insisting that control rods compensate for relatively large reactivity swings implies that large control rod penetrations would be required. This would likely result in a relatively small proportion of the fuel rods producing a large proportion of the total core power, which is generally unfavourable from a fuel performance perspective.

Erbia is usually mixed homogeneously at low concentrations within all fuel pins in an assembly since it is a relatively weak neutron absorber and depletes slowly [11]. Gadolinia on the other hand is usually mixed homogeneously within a select few pins in an assembly at high concentrations since it is a strong neutron absorber but burns out relatively quickly [11]. In the case of gadolinium Burnable Poison Pins (BPPs), typically 24 pins of the 264 fuel rods within a conventional assembly are designated BPPs [111].
Figure 3.2: Effect of altering erbia (Er$_2$O$_3$) concentration on $k_\infty$ vs time. All fuel rods contain Er$_2$O$_3$ at the designated concentrations in wt.% and a fuel density of 95% theoretical density.

(a) Assembly with 76 burnable poison pins - this layout is utilised in later assembly designs.

(b) Assembly with 96 burnable poison pins.

Figure 3.3: Location of the Burnable Poison Pins (BPPs) (in black) which contain a mixture of UO$_2$ and Gd$_2$O$_3$, and the fuel pins (in red). The layout of the BPPs was based on the fact that the reactivity, and therefore power, tends to peak in fuel rods next to the water channels where increased neutron moderation is taking place. Hence, BPPs are located in close proximity to these channels in order to try and limit power peaking in the assemblies.
(a) Reactivity profile for lattice containing 24 burnable poison pins, with differing gadolinia concentrations.

(b) Reactivity profile for lattice containing different numbers of burnable poison pins, all with 9 wt.% gadolinia concentration.

Figure 3.4: Effect of altering Gd$_2$O$_3$ concentration on $k_\infty$ vs time by burnable poison pin geometry and concentration alone. The burnable poison pin layout for lattices with 12, 24 and 48 Burnable Poison Pins (BPPs) is taken from Ref. [31]. The 96 BPP layout is shown in Figure 3.3.

Figure 3.2 shows the evolution of $k_\infty$ over time for CASMO runs containing fuel rods doped with a variety of Er$_2$O$_3$ contents. Figure 3.4 shows the equivalent lattice runs to Figure 3.2 but containing only a certain number of fuel rods doped with Gd$_2$O$_3$. The number of gadolinia doped Burnable Poison Pins (BPPs) within the 17 by 17 lattice investigated were 12, 24, 48 and 96. The burnable poison pin layout for lattices with 12, 24 and 48 Burnable Poison Pins (BPPs) was taken from Ref. [31] with the chosen 96 BPP layout shown in Figure 3.3b.

Figures 3.2 and 3.4 indicate that gadolinium exhibits a slightly lower residual poison penalty (see Section 2.6 in the previous chapter for a discussion of residual poison penalty) for a given reactivity.
profile. Besides the slightly lower residual poison penalty, there does not appear to be any major difference in their capability to control excess reactivity. However, there does appear to be significantly more experience with high gadolinia bearing fuel [38, 135, 136] compared to fuel doped with high erbia concentrations [137]. For this reason it was decided to choose gadolinia as the burnable poison to be utilised.

3.3.2 Optimisation

As the core geometry has been chosen to meet the parameters outlined in Table 3.1 and a fuel rod geometry and burnable poison selected, the radial and axial variation of burnable poison and enrichment were next to be decided on. The predominant reason for varying the poison and enrichment concentrations throughout the core was to minimise power peaking.

Choosing Lattice Contents

Firstly the precise contents of individual lattices was chosen; namely: concentration of burnable poison, number of burnable poison pins and the $^{235}$U enrichment of burnable poisons pins and fuel rods containing no burnable poison. In order to limit the number of variables a series of conditions were put in place with respect to the concentration of the chosen burnable poison (gadolinia), the number of BPPs and the $^{235}$U enrichments; these were:

1. Two distinct lattice configurations would be chosen, where a distinct lattice configuration is defined by the number of BPPs present. For instance, Figure 3.3 shows two distinct lattice configurations.

2. The concentration of Gd$_2$O$_3$ in the assembly with the greater number of BPPs would be less than the concentration in the assembly with fewer BPPs. This was because neutron flux is suppressed in BPPs, and the neighbouring fuel rods that contain no BP will be exposed to a lower neutron flux (shadowed). This will result in a reduction in the depletion rate of Gd relative to an assembly with fewer BPPs. Hence it would be unnecessary to have a much higher concentration of burnable poison in the lattice with more BPPs.

3. It is usual practice to mix high poison concentrations with lower enrichments and also to mix low poison concentrations with higher enrichments [138]. This results in relying more on the
natural depletion of fissile material to help control excess reactivity and power shaping, therefore minimising the concentration of burnable poison and the enrichment level\(^2\).

Item 1) above was imposed because of the distinct behaviour of gadolinium as a burnable poison, in that the concentration limits the reactivity swing, whereas the number of BPPs within an assembly suppresses the initial $k_{\text{eff}}$ (Figure 3.4 above illustrated this phenomenon). It was therefore decided to employ two lattice configurations, as it was assumed this would allow for some optimisation regarding suppression of the initial $k_{\text{eff}}$ and limiting the reactivity swing, whilst minimising the necessary burnable poison concentration.

In order to simplify the approach in deciding upon the appropriate lattices to employ in the final core design, so-called colourset models were constructed in CASMO. Colourset models are an infinite array of two or more lattices in a repeating pattern, similar to the layout of a checkerboard. This allows the user to quickly model the effect of using two or more different neighbouring lattices on $k_\infty$ over time. As only two distinct lattices are being considered here, the colourset models therefore contained only two distinct lattices.

Priority was given to suppressing the reactivity swing, otherwise large reactivity swings will have to be compensated by deep control rod insertions, which will likely result in a large local peaking factor (here the term local peaking factor refers to the point in space at a given time within the reactor that experiences the highest power relative to the average power of the core). As colourset models were initially used to screen potential lattice combinations, and these ignore a variety of effects including neutron leakage and thermal-hydraulic feedback, the focus was on studying how the two distinct lattice types would impact the reactivity profile.

\(^2\)Generally in PWRs it is the case that the enrichment is lower in the BPPs to reduce power peaking in $\text{Gd}_2\text{O}_3$ rods later in life, as there is greater uncertainty relating to the behaviour of high burnup BPPs relative to $\text{UO}_2$ only pins, simply because there is a far greater wealth of data for the latter. This pragmatic approach simplifies licensing of the reactor, as greater uncertainty requires larger margins in order to confidently ensure that fuel rods behave in a manner that does not result in fuel failure. However, as high gadolinium concentrations will likely be required in all BPPs (thereby reducing the uranium density, as Gd displaces U in the fuel rod) and thus effectively reducing its enrichment, all pins within an assembly will have the same enrichment.
A variety of colourset models were constructed and a summary of the results from these cases is shown in Appendix B.2. It was found that a combination of 96 and 76 BPP lattices achieved adequate suppression of the initial \( k_{\infty} \) and limited the reactivity swing. Figure 3.5 shows the lattice types that were settled on.

The next step was to take the chosen lattice configurations and implement them into a finite core using SIMULATE. When constructing the finite cores in SIMULATE the following criteria were put in place:

1. The \( k_{\infty} \) at the Beginning of Life (BOL) was chosen to be approximately 1.02;
2. At the End of Life (EOL) \( k_{\infty} \) must be greater than or equal to 1.0.

An initial neutron multiplication factor of 1.02 was chosen as in conventional reactors xenon transients can result in around 1000 pcm of negative reactivity, which in this reactor must be compensated for [139]. SIMULATE models were then constructed using different ratios of one lattice to another. It was found that employing a ratio of around two 96 BPP lattices to one 76 BPP lattice, and increasing the enrichment of both lattice types by 0.5 wt.%, resulted in reactivity profiles that met the \( k_{\infty} \) criteria at BOL and EOL.
Radial Optimisation of Core Layout

The number of unique assemblies was then increased from 2 to 6, consisting of three distinct 96 BPP lattices and three 76 BPP lattices. Initially the distinct lattices for a given type (96 BPP type or 76 BPP type) had differences of ± 1 wt.% in both enrichment and gadolinia concentration (which also ensured the enrichment/poison concentration criteria were obeyed). Therefore, for the 96 BPP lattice type, one lattice contained BPPs with 11 wt.% gadolinia and had an enrichment of 16.5 wt.% for all rods within that lattice; another lattice had 13 wt.% gadolinia and had an enrichment of 14.5 wt.%; and the final lattice of this type had 12 wt.% gadolinia and had an enrichment of 15.5 wt.%.

In order to decide upon the appropriateness of a core layout, another criterion was put in place, which was that at the start of life the assembly with the greatest relative power should be located in the central region of the core\(^3\) and that its relative power fraction should be \(\leq 1.5\), i.e. the power in the central region of the core should have the highest power share and should be \(\leq 1.5\) times the average power output of all assemblies.

![Core Layout Diagram](image)

\(\text{(a) Profile 1 core layout (initial guess).} \quad \text{(b) Profile 2 core layout (final chosen).} \)

Figure 3.6: Radial optimisation with respect to core layout was based on an initial guess for an appropriate core layout, Profile 1. The assemblies were then shuffled until a desired power profile was achieved, which was that the relative power fraction in the central region of the core, at the start of life, should be highest and be \(\leq 1.5\). Profile 2 shows the core layout that achieves the desired power profile. The colours and numbers represent assemblies IDs with their contents shown in Table 3.2.

\(^3\)The central region is defined here as the region occupied by the 9 assemblies in the centre of the core.
Figure 3.7: Radial power profiles for core layouts shown in Figures 3.6a and 3.6b at $t = 0$. Profile 1 refers to the initial guess at core layout and Profile 2 shows the settled on core layout.

Table 3.2: Breakdown of individual assembly contents. The assembly IDs correspond to those in Figure 3.6b, with the number in the assembly ID describing the number of BPPs within that assembly. Note that pins within an assembly have identical enrichment but some pins will contain burnable poison (at the concentration detailed above) and the remaining pins will consist of just $\text{UO}_2$.

Figure 3.6a shows the initial guess for the core configuration; the general trend was to put the assemblies containing higher enriched fuel nearer the outer region of the core in order to flatten the power profile at the beginning of life. Figure 3.7 shows the relative power fraction of a radial slice through row 6 of the core, for the core layout in Figure 3.6a, which corresponds to “Profile 1”. Profile 1 has a power distribution that was significantly above the targeted peak relative power fraction of 1.5. Therefore, assemblies were shuffled manually, and where necessary assemblies were replaced with other assemblies from the list of 6 unique assembly types, until the targeted profile was met and then small changes in enrichment within assemblies was made to further improve the radial power profile. This resulted in “Profile 2”, which was considered radially optimised. The corresponding core layout for Profile 2 is shown in Figure 3.6b and its $k_{\text{eff}}$ evolution is shown in Figure 3.8.

Although the adjustments in poison and enrichment concentrations by ± 1 wt.% were arbitrary, they turned out to be quite satisfactory in achieving the $k_{\text{eff}}$ evolution and power profile. No further
alterations were made to the radial loading pattern. Therefore all future cores discussed in this chapter had the same radial loading pattern as Figure 3.6b.

![Figure 3.8: $k_{eff}$ evolution for Profile 2 core layout.](image)

**Axial Poison and Enrichment Optimisation**

![Figure 3.9: Illustrating how an assembly of height $h = 245.14$ cm was split into 3 axial regions: a top Low Poison (LP) region, a middle High Poison (HP) region and a bottom LP region, in order to reduce power peaking when control rods were inserted. The colours indicate regions with the same enrichment and containing burnable poison pins with the same concentration of $\text{Gd}_2\text{O}_3$. The height of the top ($h_1$) and bottom ($h_2$) regions were to be determined.](image)

The next task was to optimise the core - with control rods inserted - by axially varying the enrichment and poison concentrations. This was because if no axial variation was employed then control rod
worth would be relatively low until rods were inserted a large fraction into the core (see Appendix B.3 for further details). Deep control rod penetration is highly problematic from a fuel performance perspective as it implies smaller regions of the core are producing disproportionately more power which could result in severe fuel degradation before the targeted core life is achieved; they also raise concerns related to Rod Ejection Accidents (see Section 3.3.3). Hence, the axial power variation was investigated whilst control rods penetrated the active region of the core. This was achieved by making alterations to the poison and enrichment variations axially across fuel assemblies. For simplicity, only three axial regions were considered: a top region, a middle region and a bottom region (within each assembly); see Figure 3.9. All rods within a region (top, middle or bottom) of a particular assembly - that is to say both fuel rods and BPPs - had the same enrichment. BPPs all had the same Gd$_2$O$_3$ concentration within each region within an assembly. Starting with the profile shown in Figure 3.6b a control rod insertion pattern was decided on and then the poison and enrichment concentrations within regions were varied.

![Figure 3.9: The Rod Control Cluster Assemblies (RCCAs) groups (banks) for the two configurations studied.](image)

Figure 3.10 shows the RCCA configurations employed. The layout in Figure 3.10a was the initial guess for an appropriate RCCA layout, which was based on the fact that PWRs usually employ one RCCA for every other assembly in a core (whereas BWRs typically employ one Control Rod Blade per assembly) and that there is a significant cost penalty associated with having many Control Rod

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Drive Mechanisms (CRDMs) that drive the RCCAs into the core [88].

Four banks of RCCAs were chosen. The banks were inserted with an offset of 10% of active core height between each bank, e.g. when the first bank was inserted 30% of the way into the core, the second bank would be inserted 20% of the way into the core, the third bank 10% and the fourth bank would just start to enter the active core region. The reasoning behind this 10% offset was because a few depletion runs with offsets between 0 and 20% showed this to be appropriate in minimising the insertion depth required to ensure criticality whilst minimising local peaking factors.

The algorithm used to calculate the necessary insertion depth of rods to ensure criticality at each time step over a burnup run preserved the bank order during insertion throughout core life, i.e. bank 1 was always inserted first, followed by bank 2, then bank 3 and finally bank 4. The 24 possible permutations of bank order at the start of core life (e.g. bank 2 inserted first, followed by bank 3, then 4 and finally bank 1 would be another permutation) were studied for the axially homogeneous core but it was found that no improvement was made on the original insertion order (bank 1 followed by bank 2 followed by bank 3 and finally bank 4). It may be possible to reduce the necessary insertion depths by permuting through the 24 possible variations of bank insertion order at various stages in core life, rather than keeping the bank insertion order fixed throughout core life. This could be investigated in future studies.

Initially large variations in axial enrichment were tried between neighbouring axial regions; these were 1, 2, 4 and 8 wt.%. Poison concentrations were also initially varied by 1, 2, 4 and 8 wt.%. In both cases poison and enrichment concentrations were kept fixed in the high poison regions of the fuel and reductions of 1, 2, 4 and 8 wt.% in burnable poison and enrichment were made to the low poison regions of fuel assemblies. Hence in total 16 (= 4×4) distinct poison and enrichment variations were made.

The other variable available was the size of the axial regions. Initially the size of the bottom (h2) region, shown in Figure 3.9, was set to the following values: 1, 5, 10, 20 and 40 cm (5 variations), and the top region of the core was set to values between 20 and 140 cm in steps of 20 cm (7 variations). This along with the poison and enrichment variations resulted in 560 (= 16×5×7) distinct cores. These

The cost penalty related to CRDMs is that because of their crucial safety function they must be engineered to very high standards to ensure they operate in a reliable fashion. Furthermore, reducing the number of CRDMs and the associated costs of installing and maintaining extra CRDMs is clearly advantageous. CRDMs also require control and sensor cables to be routed to the control room, whilst meeting stringent safety criteria such as fire protection, isolation and containment penetration. Finally, CRDMs are usually located above the vessel head, therefore more CRDMs adds to the congestion of the upper head region, increasing the difficulty of performing maintenance there [88].
cores were assessed using an algorithm that outputted which cores obeyed the following criteria:

1. A viable core must have control rods present in the active region of the core during the 15 year core life, as if control rods are removed this implies that the core was not able to sustain criticality;

2. No control rod is permitted to be inserted greater than 50% of the way into the active core region during depletion, otherwise it is likely that issues such as fuel degradation would arise if a control rod were to be ejected as the power of the assembly would increase dramatically from a very low level;

3. If conditions 1) and 2) have been obeyed then the preferred core configuration will have the smallest local peaking factor.

The algorithm used to return the number of viable cores that obey these criteria will be referred to as the discriminator algorithm. In order to speed up the run time for each core configuration initially a relatively coarse time step was used of around 1 GW.d/THM, which equates to around 70 day time steps, and the convergence criterion for $k_{\text{eff}}$ was set to $\pm 0.005$. The number of cores returned by the discriminator algorithm totalled zero, i.e. no cores had maximum control rod insertions of $< 50\%$ of core height and/or none were able to sustain criticality for the 15 year core life. It was found that a large proportion of the cores had insufficient reactivity to last for the 15 year period, which was attributed to the relatively coarse enrichment variations. Also, core configurations with a top region greater than 100 cm had very deep control rod penetrations ($> 50\%$), whereas cores with top regions shallower than 40 cm resulted in either having too little reactivity for the targeted life-time and/or large local peaking factors. Finally, there was little benefit in having a bottom region greater than 20 cm, as beyond this point cores with large local peaking factors were created, as the power distribution became heavily skewed towards the bottom of the core.

Since the first set of core combinations resulted in the discriminator algorithm returning no valid cores, a second set of axial poison and enrichment concentration variations were made to the axially homogeneous core, along with adjustments to the region sizes. This resulted in the number of cores constructed being much higher (from 560 cores to 9216). The variations were:

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5The convergence criterion in SIMULATE for $k_{\text{eff}}$ refers to point at which SIMULATE's control rod insertion algorithm will halt making adjustments to control rod insertion. For instance, as $k_{\text{eff}}$ must be equal to 1, a convergence criterion of $\pm 0.005$ will result in halting control rod movements once $k_{\text{eff}}$ falls into the range 0.995-1.005.
The range of enrichment variations was limited to $\lesssim 2$ wt.%. Enrichment variations to the HP and LP regions were 0.75, 0.5, 0 and -1 wt.%\(^6\).

- The chosen poison changes were considerably expanded and are shown in Table 3.3.

- Axial region heights were varied by 40, 60, 80 and 100 cm for the top region, with the bottom region altered by 1, 5, 10 and 20 cm.

It was decided to alter all of the HP regions together in one step in order to minimise the number of permutations. This is referred to as one group alteration and is indicated by the matching colours of cells in Table 3.3 for the HP and LP rows. For example, a variation of 3 wt.% to the BPPs in the 76 HP region resulted in a 5 wt.% alteration to the 96 HP region. The same process was applied for the LP variations but these were altered independently of the HP variations.

Therefore, as 6 poison variations were made to the HP lattice types along with 4 enrichment variations, there are 24 types of HP lattice. By the same account there are 24 LP lattice types. Next each possible HP lattice group alteration, of which there were 24, was made to the axially homogeneous core independently of the 24 LP lattice groups, resulting in 576 ($= 24 \times 24$) permutations. On top of these 576 alterations there were 16 possible axial configurations. Thus in total 9216 ($= 16 \times 576$) cores were constructed, which were subsequently analysed by the discriminator algorithm.

The ‘best’ core, resulting from the discriminator algorithm, was then run to assess Rod Ejection Accident performance (see Section 3.3.3). However, when performing rod ejection studies on the 45 RCCA configuration, it was found that greater than 1 dollar of reactivity insertion upon rod ejection

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\(^6\)A slightly larger decrease in enrichment (-1 wt.%) relative to the increase in enrichment (0.75 wt.%) was put in place as there is a preference to minimise enrichment in order to minimise fuel costs.
of the highest worth rod occurred when factoring in the usual ± 10% uncertainty used [138]. Thus, these cores failed to meet the criteria relating to rod ejection (see Section 3.3.3). Hence it was decided to increase the number of RCCAs to minimise the reactivity insertion from Hot Full Power, as it was assumed that with more rods present during power operation the effect of removing one RCCA would be smaller as the RCCAs in other assemblies would limit the increase in reactivity during the ejection of an RCCA. This is because the greater number of control rods will limit the reactivity increase of any single RCCA due to more neutron absorbing material being present. Hence, the number of RCCAs was increased from 45 to 81 as shown in Figure 3.10b (note that in total 89 assemblies are present in the core).

<table>
<thead>
<tr>
<th>Lattice key</th>
<th>Low Enrichment region (wt.%)</th>
<th>High Enrichment region (wt.%)</th>
<th>High Poison content (wt.%)</th>
<th>Low Poison content (wt.%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>96 96</td>
<td>15.5</td>
<td>17.25</td>
<td>16</td>
<td>6.75</td>
</tr>
<tr>
<td>96</td>
<td>14.5</td>
<td>16.25</td>
<td>17</td>
<td>7.75</td>
</tr>
<tr>
<td>96</td>
<td>12.5</td>
<td>14.25</td>
<td>18</td>
<td>8.75</td>
</tr>
<tr>
<td>76 76</td>
<td>11.5</td>
<td>13.25</td>
<td>18</td>
<td>10.75</td>
</tr>
<tr>
<td>76</td>
<td>10.5</td>
<td>12.25</td>
<td>19</td>
<td>11.75</td>
</tr>
<tr>
<td>76</td>
<td>9.5</td>
<td>11.25</td>
<td>20</td>
<td>12.75</td>
</tr>
</tbody>
</table>

Table 3.4: Breakdown of individual lattice contents of the optimised core. The lattice IDs correspond to those in Figure 3.6b. The high poison region that contains burnable poison pins and unpoisoned fuel pins will have enrichment at the low enrichment level, whereas the low poison region will have an enrichment at the high level specified above.

The above optimisation process was repeated for cores with 81 RCCAs and resulted in a core that complied with the rod ejection criteria put in place. Table 3.4 describes the axial poison and enrichment variation for this core. The size of the bottom axial region was 20 cm in height and the top axial region was 100 cm. As the radial profile was not being adjusted, the radial loading pattern is the same as that shown in Figure 3.6b. In the subsequent sections of this chapter this radially and axially optimised core configuration will be analysed with regards to the depth of control rods, shutdown (sub-criticality) margins, rod ejection accidents, reactivity coefficients, core behaviour with respect to temporal and spatial distribution of xenon and fuel performance.
3.3.3 Control Rod Analysis

Control Rod Heights

Figure 3.11 shows how the RCCAs move throughout core life. Note that the deepest RCCA penetration is less than 40% of core height throughout core life.

![Graph showing RCCA position as a function of core life.](image)

Figure 3.11: Variation of RCCA position as a function of core life.

Shutdown Margins

It is important that a nuclear reactor can be shut down at any point in core life. In addition, there are a number of uncertainties associated with reactor codes, due to uncertainties in nuclear data, the stochastic nature of Monte Carlo codes, and the approximations made in deterministic codes to make the neutron transport equation tractable; these must all be factored into any safety criteria such as the sub-criticality margin. This results in the concept of shutdown margins.

When analysing shutdown margins, two reactor states are normally studied: Hot Zero Power (HZP), and Cold Zero Power (CZP) with no $^{135}$Xe present. The former represents the core state once the core is initially shut down and results in the outlet temperature being equivalent to the inlet temperature, whereas the latter represents the core state many days after shutdown and results in the coolant temperature being in thermal equilibrium with its surroundings, taken here to be 20°C.

Furthermore, in order to make the calculations conservative it is normal to consider the highest worth RCCA removed (ejected) from the active region of the core during the HZP core state. This is
because it is assumed that under hot zero power conditions the core is still pressurised and it is possible that an RCCA could be ejected from the core if the mechanical housing for the RCCA were to fail and the pressurised coolant results in the rapid removal of an RCCA. However, at CZP it is possible that either a rod is accidentally removed during refuelling or an RCCA fails to enter its host assembly due to, say, some sort of mechanical deformity blocking its entry. Therefore the core reactivity was investigated with the highest worth rod also removed from the core. Normally, significant quantities of boric acid would enter the core once it is clear that shutdown will take place over an extended period of time; however, in all of the below results no boron is present in order to assess the feasibility of not requiring the addition of boric acid.

The shutdown margins are not the same for all reactor states. It is usual practice to insist on a larger shutdown margin in the CZP state as it is assumed that the reactor vessel head has been removed [138]. Therefore, if the core were to return to criticality the consequences would be far more serious as a major barrier to fission product escape (the Reactor Pressure Vessel) no longer exists.

Based on the above it was decided that the shutdown margin criteria would be:

- At HZP $k_{\text{eff}}$ must be less than 0.98;
- At CZP with no xenon present $k_{\text{eff}}$ must be less than 0.95

which are similar to those in conventional reactors [138].
Figure 3.12 shows the dependence of $k_{\text{eff}}$ over core life with 81 and 89 RCCAs fully inserted into the core apart from the highest worth RCCA, which has been fully removed. The RCCAs consisted of hybrid $\text{B}_4\text{C}/\text{Hf}$ control rods, which were made up of a Hf tip constituting 40% of rod height and the remainder being unenriched $\text{B}_4\text{C}$, as during power operation only around 40% of the rod will penetrate the active region of the core and Hf is known to exhibit superior irradiation performance (see Section 2.9 in the previous chapter).

Under HZP conditions a core consisting of 81 hybrid RCCAs is sufficient to ensure that $k_{\text{eff}}$ is less than 0.98. However, under CZP, with no xenon present, $k_{\text{eff}}$ is greater than 0.95. Increasing the number of RCCAs to 89 and ejecting the highest worth rod gave maximum $k_{\text{eff}}$s throughout life of around 0.92.

It is important to note that, besides xenon decay, reactivity will change due to a host of nuclides undergoing decay over various time periods. For instance, $^{239}\text{Np}$, with a half-life of 2.4 d, will decay to fissile $^{239}\text{Pu}$ thereby increasing core reactivity. It was found that reactivity could increase by up to around 1000 pcm once shutdown had occurred for time periods of 4000 hours in the CZP state (see Appendix B.6 for more details). Therefore, even under the CZP conditions with the highest worth RCCA ejected, $k_{\text{eff}}$ would still remain significantly below 0.95, assuming an RCCA configuration of
89 RCCAs is utilised, without requiring the addition of boric acid.

**Rod Ejection Accidents**

Rod Ejection Accidents (REA) are events where one of the housings of the Control Rod Drive Mechanisms (CRDMs) fails and, given the high internal pressure of the primary circuit, is rapidly ejected from the system over a time period of around 100 ms [140]. If the ejected rod results in a reactivity insertion sufficient to take the core to prompt criticality, i.e. the reactivity insertion is greater than 1 dollar, then there will be a rapid increase in power over a short period of time which could result in significant fuel rod failure. As a rod ejection event is very quick, and the resulting increase in core power should result in an automatic scram of the remaining RCCAs, it is currently considered virtually impossible for two rod ejection events to occur simultaneously [140].

It is possible to license a reactor system where the associated reactivity insertion of a single RCCA is greater than 1 dollar, as long as the consequences of such a large reactivity increase do not result in fuel failure, for instance at some points in core life an REA in Areva’s European Pressurised Reactor can result in greater than 1 dollar of reactivity insertion [141]. The onset of fuel failure is typically considered in terms of local fuel enthalpy (radially averaged across the pellet) being less than approximately 100 cal/g [140]. However, in order to accurately model REAs, a transient, three-dimensional, coupled neutronic and thermal-hydraulic software package, such as PARCS, would normally be employed [140]. However, as the present study is only employing steady-state codes, this is beyond the scope of this investigation. Therefore, a simpler approach, that has been used in the past [138], was to set a limit in place that the ejection of a single RCCA at Hot Full Power (HFP) should not result in a reactivity increase greater than 1 dollar.

Typically it is the case to consider the ejection of the highest worth rod from its critical rod position under HZP conditions [140], i.e. as the reactor is being brought from its shutdown state to power production. However, as rod penetrations are relatively deep during normal operation as well as the conservativeness of using a steady-state code for calculating REAs, it was believed appropriate to only consider rod ejection at HFP.
At various points in core life the highest worth RCCA of the 81 RCCAs was removed (ejected) from the core and the associated reactivity increase was calculated and compared to the margin computed by SIMULATE between delayed and prompt critical: the 1 dollar value. Figure 3.13 shows that the ejection of the highest worth RCCA at various points during core life at HFP does not result in the addition of more than 1 dollar’s worth of reactivity.

3.3.4 Reactivity Coefficients

An important characteristic of any viable core design is its stability to power changes. To ensure an inherently stable core design, the power coefficient of reactivity must be kept negative for all conceivable operating conditions. The two dominant effects in most reactors are the Doppler coefficient and Moderator Temperature Coefficient (MTC) [89]. However, when licensing a core design the whole gamut of reactivity coefficients must be studied, but to simplify analysis only the MTC and Doppler coefficient were considered here.

Typically when studying the behaviour of the MTC and Doppler coefficient, the focus is on conditions at Hot Zero Power (HZP) and Hot Full Power. The latter state is the core condition when operating at 100% of rated power. In modern PWRs the core becomes critical by the adjustment of the Soluble Boron (SB) concentration. In addition, the return to HFP is achieved by using the Reactor Coolant Pumps (RCPs) to raise the temperature of the coolant such that the inlet temper-
ature becomes approximately equal to the inlet temperature under HFP conditions. This simplifies the core design as the temperature range for a variety of reactivity coefficients has been considerably narrowed, and also simplifies the operating regime as there is a reduction in the number of variables. A marine reactor could be operated in a similar fashion to conventional PWRs but in the case of a Soluble Boron Free (SBF) design the rods would be slowly removed in order to return the core to criticality. However, there is the disadvantage of requiring an external power source in order to power the RCPs until the coolant temperature reaches HZP conditions, which adds to the capital and maintenance costs. In addition, there are other benefits attached to increasing the flexibility of being able to achieve core re-criticality at lower coolant temperatures, as it enables the reactor operator to overcome to some extent the buildup of xenon in the core. This is because at lower temperatures the core is more reactive and is able to burn out the xenon.

It was therefore decided to study four distinct temperature conditions: Cold Zero Power (CZP), Warm Zero Power (WZP), Hot Zero Power and Hot Full Power. As stated earlier, normally there is little interest in temperature conditions below HZP, however, it was decided to study a temperature condition between CZP and HZP, which was termed WZP and which had an inlet temperature of 100°C. Figures 3.14 and 3.15 show the moderator temperature and distributed Doppler coefficients respectively. The distributed Doppler coefficient refers to the case where the fuel temperature across the core has been adjusted by a temperature rise that is weighted by the core power. Further MTC and distributed Doppler coefficients were investigated at Hot Partial Power (HPP), which was assigned a core power output of 25%, in addition to reactivity coefficients at WZP and HZP at critical rod positions. These are shown in Appendix B.7.

The general trend for the MTCs shown in Figure 3.14 is that they become more negative over time, which is expected as the thermal flux increases as absorbing nuclides are burnt out. Therefore, as the spectrum softens the core becomes more sensitive to changes in moderator density as fission relies to a greater extent on thermal neutrons. However, in the case of the reactivity coefficient at HZP there is an increase in MTC later in life. Hence, additional MTC values were calculated later in life in the HZP case in order to ensure the variation in MTC was smooth rather than discontinuous, which would indicate an unphysical characteristic outputted by the code. As the MTC does not exhibit any discontinuities later in life, it was decided to investigate the cause of this unexpected behaviour. It is worth noting that in the HFP and HZP cases, the fission product inventories were unadjusted during the changes in moderator density and fuel density, as the time taken for HZP to occur is
much shorter than the time scales attributable to iodine and xenon decay. However, for a reactor’s inlet temperature to drop from 255°C to 100°C and 20°C would likely take time scales of the order of 10 hours. Therefore, in the WZP and CZP cases the inventories of iodine and xenon were set to zero. Furthermore, the HFP differs from the HZP case primarily by temperature and density of the moderator and coolant, in addition to the higher temperature. Hence, it could be argued that the reason for HZP showing different behaviour could be due to its different fission product behaviour in comparison with WZP and CZP conditions. Yet it was found that when re-running the HZP model with fission product inventories set to zero, similar MTC and Doppler coefficient evolutions were returned (a comparison of MTC and Doppler coefficients with respect to fission product inventory behaviour is also included in Appendix B.7). It was therefore decided to investigate the power profiles in these four cases as the different temperature profiles could be resulting in the unusual behaviour as the flux profiles change considerably throughout burnup.

Figure 3.16 shows the variation in Axial Offset (AO) between the four cases as a function of time. The AO is defined as the power in the top half of the core minus the power in the bottom half divided by total power. There appears to be some sensitivity to core temperature at the zero power state in the axial offset, as the axial offset is markedly different at 10 years vs 12 years which coincides with the divergent reactivity coefficients under HZP conditions. It therefore may be the case that the inventory of nuclides later on in life results in the sensitivity to coolant temperatures when all RCCAs are inserted.
Figure 3.14: Moderator Temperature Coefficient as a function of core life for Cold Zero Power, Warm Zero Power, Hot Zero Power and Hot Full Power, which correspond to coolant inlet temperatures of 20°C, 100°C, 255°C and 255°C respectively.

Figure 3.15: Distributed Doppler Coefficient as a function of core life for Cold Zero Power, Warm Zero Power, Hot Zero Power and Hot Full Power, which correspond to coolant inlet temperatures of 20°C, 100°C, 255°C and 255°C respectively.
3.3.5 Power Profiles

For completeness the radial and axial power distributions for the radially and axially optimised core are shown.

The radial power profile consistently peaks throughout life in assemblies C6 and D6 which contain RCCAs that are part of banks 4 and 2. Bank 4 is the shallowest bank throughout life and this suggests that the limited change in radial power profile is an artefact of the fixed bank insertion order. It would be preferable for the distribution in radial power profile to alter over time in order to limit the amount of power any single assembly produces throughout its life. This could be examined in future studies which investigate alternative control bank manoeuvring algorithms that attempt to further minimise
the power any one assembly produces, thereby minimising the burnup and fuel degradation of fuel rods across the core.

Figure 3.18: Power distribution of the rod with the highest burnup at end of life (located in assembly C8 in column 2 and row 17) as a function of time.

The variation in power distribution as a function of time for the rod with the highest burnup at the EOL is shown in Figure 3.18. This fuel rod was located in assembly C8.

Finally, the axial offset throughout core life is shown in Figure 3.19. The core returned by the discriminator algorithm has an axial power distribution skewed somewhat towards the top of the core as it has an average axial offset throughout life of 0.252. This implies that the power distribution is skewed towards the top half of the core throughout core life.
3.3.6 Burnup Histories

Figure 3.20 shows the range of burnups at the end of core life for all rods, showing a wide distribution in burnups. Figure B.6 shows the burnup histogram for each of the 16 distinct assemblies in one octant of the core. It was found that rods in the peripheral assemblies (in columns A, B and to some extent C - see Figure 3.6b) create this large distribution as they have a significant fraction of rods achieving burnups of less than 40 GW.d/tHM (see Appendix B.5). Radially optimising the burnable poison and enrichment (in addition to a more refined control rod search algorithm) would very likely considerably reduce the peripheral assemblies’ poor burnup distribution and could be performed in future studies.

![Histogram of individual rod burnups across the entire core](image)

Figure 3.20: Histogram of individual rod burnups across the entire core, with the blue histograms indicating the burnup of burnable poison pins and the transparent histograms showing the burnup of fuel pins (rods containing no burnable poison).

3.3.7 Xenon Fission Product Effects

Xenon Transients

$^{135}\text{Xe}$ is the most important fission product due to its very large thermal absorption cross-section (2.7 Mb vs 700 b for $^{235}\text{U}$) and its relative high fission product yield. Other important characteristics are that $^{135}\text{Xe}$ is produced both directly as a fission product (yield $\approx 0.2\%$) and indirectly via decay from $^{135}\text{I}$ (yield $\approx 6\%$). $^{135}\text{Xe}$ and $^{135}\text{I}$ also differ in their decay constants, which are 0.10 hr$^{-1}$ and 0.08 hr$^{-1}$ respectively. These properties imply time dependent behaviour on flux variations. From this point forward, xenon and iodine will refer to $^{135}\text{Xe}$ and $^{135}\text{I}$ respectively.

In conventional LWRs, so-called xenon transients complicate startup, shutdown and power level
changes. In the case of reactor shutdown, $^{135}$Xe will initially build up as the destruction mechanism of $^{135}$Xe to $^{136}$Xe is no longer available due to zero neutron flux, and the inventory of $^{135}$I will decay to $^{135}$Xe. The increase in $^{135}$Xe concentration implies that excess reactivity will be required to achieve re-criticality, as the inventory of $^{135}$Xe increases up until the point where the predominant mechanism determining $^{135}$Xe concentration is the decay of this isotope. Xenon transients are usually overcome using chemical reactivity control (i.e. adjustment in soluble poison concentration) and most reactors world-wide operate at fixed power levels, therefore xenon transients are only normally problematic in unplanned outages. However, for a marine reactor, there is no scope to operate the reactor at a fixed power level as the ship will enter port on a relatively frequent basis and the power level will need to be decreased. Therefore the behaviour of the core with power level changes was studied.

Xenon transients were initiated in the simulation by inserting all 81 RCCAs into the core, resulting in HZP conditions, and then tracking the xenon and iodine concentrations in SIMULATE over a time period of 20 hours with time steps of 0.2 hours. The minimum $k_{\text{eff}}$ value could then be found, in order to determine the reactivity decrement associated with xenon. Table 3.5 shows the negative reactivity insertion associated with xenon transients taking place at various points in core life. Earlier it was stated that typically xenon transients are of the order 1000 pcm [139], therefore the reactivity effect of xenon transients is very small.

<table>
<thead>
<tr>
<th>Time transient initiated</th>
<th>Peak Xe time</th>
<th>Associated reactivity decrement</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 d</td>
<td>1.6 h</td>
<td>-6 pcm</td>
</tr>
<tr>
<td>4.90 y</td>
<td>1.8 h</td>
<td>-11 pcm</td>
</tr>
<tr>
<td>10.0 y</td>
<td>1.6 h</td>
<td>-10 pcm</td>
</tr>
<tr>
<td>15.0 y</td>
<td>3 h</td>
<td>-38 pcm</td>
</tr>
</tbody>
</table>

Table 3.5: Details the negative reactivity insertion associated with xenon transients taking place at various points in core life under Hot Zero Power conditions.

The reasoning behind this core’s relative insensitivity to xenon transients turned out to be the very limited swing in xenon concentration over the course of the transient. Figure 3.21 shows the change in xenon and iodine concentrations as the transient progresses at the end of core life. Appendix B.8 includes plots of xenon concentration over the course of the transient for the various transient times shown in Table 3.5.
Normally in PWRs the iodine concentration at hot full power is higher than the xenon concentration for a number of reasons. One is that the majority of the $^{135}$Xe present within the reactor is from the decay $^{135}$I to $^{135}$Xe. In addition, a significant proportion of the xenon is destroyed by thermal neutrons, whereas $^{135}$I has a much smaller thermal absorption cross-section compared to $^{135}$Xe. Therefore, as the power level drops, the xenon concentration increases over time scales comparable to the half-life of $^{135}$I as the iodine decays into $^{135}$Xe. However, the above description is only valid at certain fluxes. This can be shown by using the $^{135}$Xe and $^{135}$I concentration equations, which are

$$\frac{dX}{dt} = \lambda_I I + \gamma_X \Sigma_f \phi - \lambda_X X - \sigma_X \phi X$$  \hspace{1cm} (3.3)$$
and

$$\frac{dI}{dt} = -\lambda_I I - \sigma_I \phi I + \gamma_I \Sigma_f \phi$$  \hspace{1cm} (3.4)$$

where $\lambda_I$ and $\lambda_X$ are the decay constants for $^{135}$I and $^{135}$Xe respectively, $\sigma_I$ and $\sigma_X$ are the microscopic thermal absorption neutron cross-sections for $^{135}$I and $^{135}$Xe respectively, $\phi$ is the thermal flux, $\gamma_I$ and $\gamma_X$ are the fission product yields for $^{135}$I and $^{135}$Xe respectively and $\Sigma_f$ is the macroscopic thermal neutron cross-section for fission of the fuel material in the reactor.

Equation 3.4 can be simplified by noting that the term $-\sigma_I \phi I$ is negligible in comparison to the other terms given that the microscopic cross-section for $^{135}$I is around $7 \times 10^{-24}\text{cm}^2$. Therefore equation 3.4 becomes

$$\frac{dI}{dt} = -\lambda_I I + \gamma_I \Sigma_f \phi.$$  \hspace{1cm} (3.5)$$
From Equations 3.3 and 3.5 the equilibrium $^{135}\text{I}$ ($I_0$) and $^{135}\text{Xe}$ ($X_0$) concentrations are

$$I_0 = \gamma_I \Sigma_f \phi_0 / \lambda_I$$

(3.6)

and

$$X_0 = (\lambda_I I_0 + \gamma_X \Sigma_f \phi_0) / (\lambda_X + \sigma_X \phi_0)$$

(3.7)

Solving Equations 3.6 and 3.7 for the case where $I_0 < X_0$, gives $\phi_0 < 2.9 \times 10^{12}$ using values of $2.9 \times 10^{-5} \text{s}^{-1}$, $2.1 \times 10^{-5} \text{s}^{-1}$, $0.003$, $0.056$ and $3.5 \times 10^{-18} \text{cm}^2$ for $\lambda_I$, $\lambda_X$, $\gamma_X$, $\gamma_I$ and $\sigma_X$ respectively.

Therefore, at thermal fluxes of less than around $10^{12} \text{ns}^{-1} \text{cm}^{-2}$ the iodine equilibrium concentration is less than the xenon concentration. The average thermal flux across the core within this reactor at end of life, calculated by SIMULATE, was found to be around $6 \times 10^{12} \text{ns}^{-1} \text{cm}^{-2}$. For large PWRs the thermal flux is typically of the order of $10^{14} \text{ns}^{-1} \text{cm}^{-2}$. However, this reactor differs significantly in a number of ways. Firstly, the enrichment is much higher than in conventional PWRs (around three times higher) and the power density is roughly one third of normal PWRs; these two characteristics explain the much lower thermal flux for this reactor design relative to conventional PWRs.

Figure 3.22 shows the change in thermal flux over core life. The flux softens due to depletion of fissile material and burnable poison over the 15 year period. The larger thermal flux at the EOL relative to BOL helps explain the larger sensitivity to xenon at EOL shown in Table 3.5, as xenon is a strong thermal absorber.

![Figure 3.22: Thermal flux as a function of time.](image)
As the effect of xenon transients on core reactivity increases there will come a point in core life where the core will no longer be able to sustain criticality. It was found that beyond 14.25 years the core could no longer overcome the xenon transients attributable to HZP to HFP at peak xenon because the reactivity margin was too small. There are few options available to overcome xenon transients later in life; one would be to simply wait for xenon to decay, another would be to lower the reactor power such that peak xenon concentration is reduced and a final option would be to start the reactor at a lower temperature than HZP. This latter option allows the reactor operator to gain from the increased core reactivity at lower coolant temperatures.

Another criterion that arises relating to xenon transients is that as the reactor returns to power the remaining xenon will initially be destroyed by the neutron flux, thereby decreasing xenon concentration and increasing reactivity. The xenon concentration will eventually increase and reach its equilibrium level, which results in a decrease in reactivity. The RCCAs must therefore be able to compensate for this and hence move in step with the change in xenon concentration, which places certain criteria regarding rod movement speeds. However, as the core in this study has small differences between equilibrium and peak xenon this is very unlikely to result in any prohibitive requirements. In fact, when studying movement requirements using SIMULATE’s control rod movement algorithm under HFP conditions the maximum rod movements were around 0.2 cm per minute. It should be considered, however, that the $k_{\text{eff}}$ convergence criterion was relatively large, 250 pcm, in comparison to xenon reactivity effects, which were of the order of 10 pcm. This therefore limits the resolution of any analysis relating to rod movement to compensate for changes in xenon concentrations. Nonetheless, it does show that the effect of xenon on rod movement requirements is likely to be very small.

### 3.3.8 Xenon Oscillations

Besides overall core reactivity changes, the dependence of $^{135}\text{Xe}$ on flux also creates the possibility for localised variations in $^{135}\text{Xe}$ concentration within the core, which can lead to so-called xenon oscillations. Xenon oscillations occur due to perturbations in the flux within a reactor [89]. Consider for instance that the core is operating at constant power and a control system is present to ensure power output is fixed. Therefore in the event that flux is decreased in one region of the core, for example because a single control rod cluster has been dropped into the core, the flux must increase in a neighbouring region in order to keep the power at a constant level. The increase in flux in one region of the core causes an instantaneous decrease in $^{135}\text{Xe}$ concentration within that region due to
the transmutation of $^{135}$Xe to $^{136}$Xe. Similarly the $^{135}$Xe concentration in the perturbed region will increase due to fewer neutrons available to destroy $^{135}$Xe. Furthermore, this perturbation is unstable as an increase in flux destroying absorbing $^{135}$Xe will consequently cause an increase in flux therefore destroying more $^{135}$Xe. These effects can cause a large flux gradient to exist between neighbouring regions. This process is limited, however, by the finite pool of $^{135}$Xe (once all $^{135}$Xe is destroyed there is no more $^{135}$Xe to transmute) and the high flux gradient itself, which creates a larger current to carry excess neutrons to neighbouring regions. In time, the high flux side, with a corresponding higher reactivity and therefore greater number of fission events, will have a correspondingly higher amount of $^{135}$I, which has a half-life of 6.7 hours. Hence, the $^{135}$Xe inventory will start to increase in the high flux side and will also decrease in the low flux perturbed region as its reactivity would have been lower and therefore have fewer fission events to generate $^{135}$I. Therefore, the flux gradient will reverse and produce a side-to-side oscillation.

The main problem relating to xenon-induced spatial oscillations is its effect on local peaking factors, which if not factored into the design could lead to fuel failure [142]. Given that this core has already rather high local peaking factors, xenon oscillations could exacerbate this issue\textsuperscript{7}. Therefore a series of cases were constructed in order to find the susceptibility of the reactor to xenon oscillations.

Firstly, axial xenon oscillations were studied by inserting the lead bank of RCCAs into the core by 50%, with all other banks removed from the core. The lead bank was left inserted for 20 hours in order to ensure equilibrium xenon had been reached. The RCCAs were then subsequently removed and the Axial Offset (AO) was then followed for 20 hours. Figure 3.23 details the results of trying to initialise an axial xenon oscillation at various points in time along core life.

\textsuperscript{7}The local peaking factors in the core designed in this study are around twice as high as local peaking factors in conventional PWRs that utilise soluble boron [143].
Figure 3.23: Axial offset behaviour after only bank 1 RCCAs were inserted to core, to a depth of 50%, for the period from $t = -20$ hours to $t = 0$ hours and then fully removed resulting in no rods in the active core region.

Early on in core life there is little dependence of AO evolution with burnup, however, after approximately 10 years the AO does become more sensitive. There are two reasons for this: 1) the core will become more sensitive to xenon as the flux softens; 2) how much overlap there is between the xenon distribution after the transient in comparison to the flux distribution. The latter point is particularly important as if the flux distribution (once the rods are removed) is comparable to the xenon distribution then the xenon will have a greater effect as it encounters more neutrons to absorb.

In all cases the xenon naturally shifts towards the bottom of the core, but will then follow the flux profile and will finally return to a distribution that is similar to the one before the transient took place. This generally implies an increase in xenon concentration towards the top of the core relative to its position just before the rods are removed. The result of this is for reactivity to decrease in the top portion of the core and hence the AO decreases.

Finally, attempts were made to initiate radial xenon oscillations. This was carried out by removing all RCCAs but leaving a single RCCA fully inserted. The core was subsequently depleted for 20 hours and the RCCA was then removed. A sample of RCCAs were individually dropped into the core at various points along core life. Radial xenon oscillations are more likely in cases where RCCAs are inserted near the periphery of the core, therefore the sample of RCCAs were: A06, A07, B06, B07, B08, C06, C07, C08 and C09.

Once the RCCA was removed the Relative Power Fraction (RPF) in the opposite quadrant was recorded to see how the radial power varied over a 60 hour period. The Quadrant RPF is defined here as the power of one quadrant divided by the average power of all quadrants. As was the case with
the axial xenon oscillation investigation, transients were initiated at \( t = 10 \) days, 5 years, 10 years and 15 years. All oscillations decayed away over the 60 hour period, i.e. the ejection of the sampled RCCAs did not result in any self-propagating xenon oscillation. Figure 3.24 shows the oscillation with the largest amplitude at any point over the course of the transient; this was the ejection of RCCA B06 at \( t = 5 \) years. As can be seen, the difference in RPF is minimal (<2%) and rapidly decays away.

![Figure 3.24: Radial xenon oscillation profile associated with the ejection of RCCA B06 at \( t = 5 \) years, which had the largest largest oscillation amplitude of any xenon radial oscillation studied.](image)

The core design thus appears to be robust against xenon induced oscillations as perturbations are unsuccessful in setting up self-sustaining xenon oscillations. There are numerous reasons for this including the strong negative moderator temperature coefficient (as no soluble boron is present), in particular later on in life when flux becomes more thermalised and therefore more susceptible to xenon oscillations - clearly a further advantage to operating without soluble boron. The stronger reactivity feedback implies smaller differences in reactivity between neighbouring regions and therefore flux gradients and the difference between \(^{135}\text{Xe}\) and \(^{135}\text{I}\) concentrations are reduced. Xenon oscillations become more noticeable as core size increases; this is because they are related to the degree of de-coupling between neighbouring regions\(^8\), therefore it is to be expected that a smaller core will be less susceptible to xenon oscillations. However, probably the largest contributor to the lack of sensitivity to perturbations is the small thermal flux of the core as this limits the difference between xenon and iodine concentrations as shown when studying xenon transients. Also this helps limit the effect of the weaker moderator temperature coefficient at the beginning of life, which would be expected to make the core more sensitive to variations in \(^{135}\text{Xe}\) and \(^{135}\text{I}\) concentrations; however, the low initial core

\(^8\)Xenon oscillations are only possible in a reactor with linear dimensions around 30 times greater than the thermal neutron migration length (which is 0.059 m in light water at 293 K) [89, 142]. This is because in smaller systems the neutrons readily diffuse directly from one region to another, thus limiting the effect of the flux gradients necessary for spatial oscillations to occur [142].
thermal flux significantly reduces the ability for large increases in $^{135}$Xe concentration to occur.

### 3.4 MONK Analysis

It was decided to firstly compare MONK with an isothermal SIMULATE run, i.e. outlet temperature equal to the inlet temperature and the fuel temperature set to the coolant temperature. This simplifies the comparison between MONK and SIMULATE as MONK version 9A currently only contains temperature data on uranium isotopes up to 900 K and gadolinium data at 293.16 K, whereas SIMULATE-3 (using data supplied from CASMO-4 runs) is able to consider higher fuel temperatures. Furthermore, the control rods were also removed from the models in order to validate the agreement between SIMULATE and MONK before rods were inserted. The MONK model also has fewer axial regions than the SIMULATE model (9 vs 16); it was found that for the purposes of calculating $k_{\text{eff}}$ as a function of burnup, 9 axial regions were sufficient to ensure adequate statistics in a timely manner without introducing any significant bias due to a coarser mesh size (see Appendix B.9.2 for more details).

![Graph comparing MONK and SIMULATE results](image)

**Figure 3.25**: MONK vs SIMULATE results under isothermal conditions using nuclear data libraries based on JEF 2.2 nuclear data. The shaded region corresponds to a deviation of $\pm 1\%$ from the returned $k_{\text{eff}}$ value at each time step from MONK.

Figure 3.25 compares the results from the MONK calculation with SIMULATE. The MONK results include a shaded region constituting a deviation of $\pm 1\%$ from the returned $k_{\text{eff}}$ value at each time step in order to aid in comparing the extent of the discrepancy between MONK and SIMULATE results. Note that in MONK the standard deviation convergence at each time step was set to $\pm 0.001$, which
was found to ensure adequate statistics throughout core life.

As will be discussed in Chapter 5, the discrepancies in $k_{\text{eff}}$ between Monte Carlo codes and deterministic codes in reactor physics applications for the lattices used in commercial reactors (i.e. LEU fuel contained in relatively thin pins) are usually <0.5%. A 1% discrepancy is not atypical for unusual lattice configurations, for example this reactor which uses large amounts of burnable poison and where enrichment is approximately 3 times that of normal PWRs. However, Figure 3.25 shows discrepancies larger than this at various points in core life, whilst showing very small discrepancies at the very beginning of core life.

In order to understand what was causing the change in discrepancy between MONK and SIMULATE as a function of time it was important to understand what the main differences were between conventional PWRs, for which CASMO/SIMULATE are well validated, and the reactor being investigated in this study. The most unusual attribute of the reactor designed in this study - in comparison to conventional PWRs - is probably its relatively low thermal flux, which changes considerably over time as the strong thermal neutron absorbing nuclides of gadolinium and uranium are depleted (recall Figure 3.22). In order to gain some understanding of what might be causing the discrepancy, it was decided to compare three simple cases:

1. UO$_2$ fuel pins containing 5 wt.% $^{235}$U surrounded by unborated light water.
2. UO$_2$ fuel pins containing 13.5 wt.% $^{235}$U surrounded by unborated light water.
3. UO$_2$ fuel pins containing 13.5 wt.% $^{235}$U in addition to 76 pins containing 12.75 wt.% Gd$_2$O$_3$ surrounded by unborated light water.

All three cases had the same geometry as the lattices used in the core designed in this study (e.g. same pellet dimensions, clad thickness, etc.). Three cases were investigated as Case 1 is comparable to lattices in conventional PWRs, which both MONK and CASMO-SIMULATE are well validated for; Case 2 contains fuel pins with comparable enrichment to the lattices in this investigation; and finally Case 3 has lattice contents representative of the lattices in the marine reactor core at the BOL. All three cases were run at conditions representative of hot zero power, cold zero power and a further case where the moderator temperature was set to 293 K but fuel temperature set to 528 K. This final sub-case allows for the dependence of neutron multiplication factor on fuel temperature to be investigated. The results from these nine scenarios are shown in Table 3.6. Mirror boundary
conditions were declared in the MONK runs to ensure that the boundary conditions in both MONK and CASMO were identical. In addition, whilst both CASMO and MONK were run using the same nuclear data library (JEF 2.2), they are not in a consistent format as CASMO-4 utilises a 70 group structure to store the data whereas burnup calculations in MONK 9A necessitate the use of the WIMS 172 group structure.

<table>
<thead>
<tr>
<th>Case ID</th>
<th>Description</th>
<th>MONK $k_\infty$</th>
<th>CASMO $k_\infty$</th>
<th>Discrepancy (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1A</td>
<td>$T_{\text{moderator}} = T_{\text{fuel}} = 528 \text{ K}$</td>
<td>$1.45088 \pm 0.00027$</td>
<td>$1.44152$</td>
<td>$0.649 \pm 0.019$</td>
</tr>
<tr>
<td>1B</td>
<td>$T_{\text{moderator}} = T_{\text{fuel}} = 293 \text{ K}$</td>
<td>$1.49480 \pm 0.00015$</td>
<td>$1.48684$</td>
<td>$0.535 \pm 0.010$</td>
</tr>
<tr>
<td>1C</td>
<td>$T_{\text{moderator}} = 293 \text{ K}$ and $T_{\text{fuel}} = 528 \text{ K}$</td>
<td>$1.48444 \pm 0.00043$</td>
<td>$1.47618$</td>
<td>$0.560 \pm 0.029$</td>
</tr>
<tr>
<td>2A</td>
<td>$T_{\text{moderator}} = T_{\text{fuel}} = 528 \text{ K}$</td>
<td>$1.56624 \pm 0.00027$</td>
<td>$1.54873$</td>
<td>$1.13 \pm 0.17$</td>
</tr>
<tr>
<td>2B</td>
<td>$T_{\text{moderator}} = T_{\text{fuel}} = 293 \text{ K}$</td>
<td>$1.61374 \pm 0.00024$</td>
<td>$1.59869$</td>
<td>$0.941 \pm 0.015$</td>
</tr>
<tr>
<td>2C</td>
<td>$T_{\text{moderator}} = 293 \text{ K}$ and $T_{\text{fuel}} = 528 \text{ K}$</td>
<td>$1.60342 \pm 0.00031$</td>
<td>$1.58705$</td>
<td>$1.03 \pm 0.02$</td>
</tr>
<tr>
<td>3A</td>
<td>$T_{\text{moderator}} = T_{\text{fuel}} = 528 \text{ K}$</td>
<td>$1.10928 \pm 0.00021$</td>
<td>$1.10816$</td>
<td>$0.101 \pm 0.014$</td>
</tr>
<tr>
<td>3B</td>
<td>$T_{\text{moderator}} = T_{\text{fuel}} = 293 \text{ K}$</td>
<td>$1.13340 \pm 0.00031$</td>
<td>$1.13427$</td>
<td>$-0.077 \pm 0.027$</td>
</tr>
<tr>
<td>3C</td>
<td>$T_{\text{moderator}} = 293 \text{ K}$ and $T_{\text{fuel}} = 528 \text{ K}$</td>
<td>$1.12768 \pm 0.00015$</td>
<td>$1.12606$</td>
<td>$0.144 \pm 0.013$</td>
</tr>
</tbody>
</table>

Table 3.6: Discrepancy between the $k_{\infty}$s from MONK 9A (using 172 group nuclear data library based on JEF 2.2 nuclear data) and CASMO-4 (using a 70 group nuclear data library based on JEF 2.2 nuclear data) runs for three separate lattice configurations (differing in enrichment and burnable poison concentrations), subdivided into three further cases to assess the sensitivity to fuel and moderator temperatures. Lattices are the 17 by 17 assemblies being investigated in this study.

In all of the cases shown in Table 3.6, the uncertainty associated with the Monte Carlo runs is sufficiently small that any discrepancy between MONK and CASMO is extremely unlikely to be a result of the statistical nature of the Monte Carlo method. In the cases containing no burnable poison there is clearly some sensitivity to neutron spectra, as the addition of higher $^{235}$U enrichment will reduce the number of thermal neutrons, and also as temperature increases the general trend is for the discrepancy to increase.

In order to try and understand why the poisoned and unpoisoned 13.5 wt.% enriched lattices differ
Table 3.7: Assessing 3 cases from Table 3.6 - which were representative of Hot Zero Power conditions in the core designed in this study - by spectrum type using the metric $k_{\text{fast}}/k_{\text{total}}$. This metric is used to quantify the hardness of the spectrum relative to conventional (highly thermalised) PWR lattices, for which SIMULATE and MONK are well validated and the discrepancy is known to be small. In conventional PWR lattices the contribution of $k_{\text{fast}}$ to $k_{\text{total}}$ is typically around 0.2\cite{15}, which is similar to the value shown for Case 1A. However, clearly Cases 2A and 3A depart dramatically from this value; this indicates that different spectra may be causing the discrepancy shown in Table 3.6.

so greatly an attempt was made to quantify the hardness of the spectrum at different points in time. The parameter employed was $k_{\text{fast}}/k_{\text{total}}$, where $k_{\text{total}} = k_{\text{fast}} + k_{\text{thermal}} \text{.}\footnote{In CASMO-4, $k_{\text{fast}}$ and $k_{\text{thermal}}$ are defined as the contributions to $k_\infty$ by neutrons with energies $\geq 4$ eV and $< 4$ eV respectively. $k_\infty = \frac{\sum_g \Sigma_{f,i}^g \phi_i^g V_i}{\sum_g \Sigma_{a,i}^g \phi_i^g V_i}$, where $\nu$ is the number of neutrons released per fission, $\phi_i^g$ is the flux within mesh $i$ and group $g$, $V_i$ is the volume of mesh $i$, $\Sigma_{f,i}^g$ is the macroscopic fission cross-section of mesh $i$ and group $g$ and $\Sigma_{a,i}^g$ is the macroscopic absorption cross-section of mesh $i$ and group $g.$}$ Table 3.7 shows how Cases 1A, 2A and 3A differ in their values of this parameter - Cases 1A, 2A and 3A were investigated further as these are lattices based on the conditions in the MONK depletion run in Figure 3.25, i.e. inlet temperature equal to the outlet temperature and the fuel temperature set to the coolant temperature. Table 3.7 helps explain the difference between Cases 2A to 2C and 3A to 3C, in that 3A’s $k_{\text{eff}}$ is significantly more dominated by $k_{\text{fast}}$ in comparison to 2A, whilst 1A is the only case where $k_{\text{thermal}}$ dominates by a large margin.

A selection of cases from Table 3.6 were run using the BINGO library format in MONK (once again utilising JEF 2.2 nuclear data) which stores the data in a continuous format, i.e. it is not stored in a coarse group structure. This permits the results in Table 3.6 to be studied with regards to their sensitivity to the nuclear data structure.

<table>
<thead>
<tr>
<th>Case</th>
<th>MONK $k_\infty$ (BINGO)</th>
<th>Discrepancy (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1A</td>
<td>1.45122 ± 0.00008</td>
<td>0.673 ± 0.006</td>
</tr>
<tr>
<td>2A</td>
<td>1.56552 ± 0.00017</td>
<td>1.084 ± 0.011</td>
</tr>
<tr>
<td>3A</td>
<td>1.12174 ± 0.00019</td>
<td>1.225 ± 0.017</td>
</tr>
</tbody>
</table>

Table 3.8: Discrepancy between CASMO-4 and MONK 9A when employing the BINGO (continuous) nuclear data structure compared to the 70 group library employed in CASMO-4, both using JEF 2.2 nuclear data.
deviations of one another. However, the discrepancies for Cases 2A and 3A are not comparable as the discrepancies in results are in both cases greater than $2\sigma$, in particular the discrepancy is significantly larger for Case 3A. This implies that the reason for the similarity between CASMO-4 and MONK 9A using the WIMS 172 group library structure for Cases 3A to 3C is in part due to error cancellation that occurs because of the coarse library structure in MONK using the WIMS 172 group structure when the spectrum is dominated by high neutron energies, rather than CASMO-4 being able to accurately model systems where the reactivity is dominated by the $k_{\text{fast}}$ term. Appendix B.11 includes data on the flux spectra for Cases 1A and 3A.

Ideally we would like studies comparing CASMO-4 and MONK-9A results with experimental lattices representative of the ones in Table 3.6, which can then be used as a proxy for lattices of interest for this particular core. Unfortunately there are few experiments available at $^{235}\text{U}$ concentration above around 10 wt.% but below 20 wt.% to benchmark CASMO and MONK against and therefore it is difficult to say with high confidence which code is more accurate. However, the inherent ability of Monte Carlo codes to more accurately represent the nuclear data and flux spectrum throughout life results in a preference to regard MONK’s results using the continuous BINGO library format as less prone to systematic bias.

As stated before, discrepancies of greater than 1% between Monte Carlo and deterministic codes are generally considered large and would certainly bring into question the ability to confidently predict the behaviour of the core throughout life and therefore license the core design. However, as this study is only preliminary and is focused on the general physical behaviour of the core over core life (such as xenon transient behaviour), this large uncertainty does not significantly degrade the worth of this investigation. It does, however, highlight that deterministic codes will require modification to accurately predict the behaviour of the core. Also, a significant amount of experimental work will need to be carried out in order to obtain the data to validate codes.

### 3.4.1 Modelling Epithermal Systems

The core designed in this study has a relatively high enrichment ($>10$ wt.%) and a high poison loading, which results in a hardened spectrum during a large part of the core’s life. Therefore the core is perhaps best described as an epithermal system.

There are a number of deficiencies in thermal lattice codes with respect to modelling epithermal systems; namely:
• The limited number of energy groups;

• The structure of these energy groups;

• The approximation of the neutron flux used at the beginning of the calculation to determine multi-group constants (see Section 3.2.1).

CASMO-4 utilises a relatively coarse 70 group energy structure with 44 of these groups below 10 eV, and therefore utilises only 26 energy groups to describe neutrons in the range $10^7$ eV to 10 eV. Hence, not only is the overall number of groups limited but the structure of these energy groups is biased towards low energy neutrons. Whilst such a group scheme is reasonable for lattices with a relatively large number of neutrons at thermal energies that contribute significantly to the overall reactivity of the system, it is very likely that such a group scheme is inappropriate for a core which has an epithermal flux distribution.

In addition to the poor suitability of the energy group scheme in CASMO-4, there is also the fact that the multi-group constants used at the beginning of the calculation are based on the assumption that flux has a distribution comparable to those found in conventional PWRs. This will be inappropriate for the core in this study, especially at the beginning of life.

Fast reactor codes typically utilise around 2000 energy groups [144]; however, it would be inappropriate to utilise a fast reactor code for modelling the lattices in the core designed in this study. This is because fast reactor codes effectively ignore the behaviour of neutrons with very low neutron energies ($\lesssim 10$ eV). These low energy neutrons still play a significant role in the core designed in this study as they contribute around 50% towards the overall reactivity of the core (see Table 3.7). Ideally, a code would be created that specifically targets the deficiencies in thermal lattice codes outlined above. In the meantime however, it would be advisable for future studies to run the system’s lattices through a code using a more detailed group structure (CASMO-5 for instance makes use of 586 groups with 169 groups covering the range $10^7$ eV to around 10 eV, which compares to CASMO-4 utilising 26 groups in this energy range [145]), which may reduce the discrepancy as the flux can be more accurately determined in the higher energy region.
3.5 Fuel Performance

This section focuses on assessing the fuel performance of sampled rods within the current core design. In addition, attempts are made to highlight deficiencies in current understanding of various fuel phenomena that result in difficulties trying to accurately predict fuel rod behaviour due to the unique characteristics of the core in this study relative to fuel rods in conventional PWRs.

3.5.1 Fuel Performance of Rod Samples

The primary aim when carrying out fuel performance calculations is to ensure that the fuel does not operate outside of its design regime, i.e. it does not fail under normal operation conditions and transients due to ‘frequent’ faults, such as increased power demand resulting from a turbine trip. It is important to note that in reactor licensing ‘frequent’ is generally defined as having a probability of occurrence greater than $1 \times 10^{-3}$ per year [146].

Besides clad corrosion\(^\text{10}\) the two predominant criteria fuel rods must avoid are:

- High rod internal pressure due to a substantial inventory of fission gases that have escaped the fuel matrix;
- Large clad hoop creep strain, predominantly caused by pellet swelling as burnup increases.

The rod internal pressure is usually limited to being below the coolant pressure, which is 15.5 MPa [134]. This is because of the possibility that if the rod internal pressure is sufficiently high then the pellet-clad gap could re-open. Over time the initial pellet-clad gap will shrink in size due to a variety of phenomena including the fact that fuel pellets swell as they burn up. However, if the gap were to re-open later in a rod’s life then this could quickly lead to clad rupture, due to the fact that the thermal conductivity across the re-opened gap will be heavily degraded by the presence of gaseous fission products Xe and Kr. Both Xe and Kr possess very low thermal conductivities and therefore a large temperature gradient across the re-opened gap can arise. This can result in excessive pellet temperatures, which accelerates the release of Xe and Kr from the fuel matrix, hence further degrading the thermal conductivity of the re-opened pellet-clad gap and increasing the temperature of the fuel, thus releasing more fission gas. Eventually the rod will rupture if its internal pressure becomes

\(^{10}\)Corrosion performance will not be studied directly here as it is assumed that insisting on maximum clad external surface temperatures below $310^\circ$C will ensure the survivability of the fuel rod from a corrosion perspective (see Section 2.7.3 in the previous chapter).
sufficiently high due to the large inventory of gaseous fission products. With respect to the clad hoop creep strain, a limit of 1% is usually put in place [17] to ensure that the likelihood of clad rupture, due to time dependent plastic deformation, is very low.

As the core designed in this study consists of conventional rods, albeit with slightly fatter pellets, this constituted an initial guess for the necessary fuel rod geometry to ensure no fuel rod failure. That is to say, the rods are taken to be solid (non-annular) pellets, with an initial pellet-clad gap \(8.2 \times 10^{-3}\) cm and a plenum at the top and bottom of the fuel rod (to accommodate fission gases) of 25.40 cm (10 inches) in length (14.53 cm\(^3\))\(^{11}\). Therefore, the designer usually has three variables to adjust\(^{12}\):

1. Initial pellet-clad gap size;
2. The pellet radial geometry (annular or non-annular);
3. Plenum length.

Table 3.9 shows the rods that were sampled and the effect of adjusting these parameters on fuel performance. Note that the first two characters in ‘Pin ID’ refers to the assembly location, e.g. F6 would refer to the central assembly, and the four remaining digits are the rod location within that assembly with the bottom left corner taken as the origin so that 0101 would refer to rods located in the bottom left corner.

Firstly, it was decided to store burnup histories from SIMULATE in discretised intervals and then sample the highest burnup rods in each bin. The burnup of the rod with the highest average burnup along its length was approximately 125 GW.d/tHM, therefore the intervals chosen were 125, 115, 100, 85, 60 and 40 GW.d/tHM with smaller bin sizes for the highest rod burnups as these were assumed more likely to suffer failure. No rods below 40 GW.d/tHM were analysed as it was thought that the burnup for these rods was sufficiently low that rod failure was unlikely to occur. It is worth pointing out here that a rod with a mean burnup along its length at the end of life (EOL) of 125 GW.d/tHM is very high for LWR fuel and is sometimes referred to as ultra-high rod burnup, as the burnup has

\(^{11}\)Typically fuel rods only incorporate a single plenum with a length of less than around 9 inches [147]. Some newer fuel designs incorporate a plenum at the top and the bottom of the core [148]. Therefore here it has been assumed that two slightly larger plenums have been incorporated at the bottom and top of the rod, as the inevitable high burnup will necessitate a greater volume to accommodate the higher inventory of fission gasses.

\(^{12}\)In principle the thickness of the clad can also be adjusted, but usually this is avoided as there is a preference to minimise the clad thickness to minimise parasitic neutron absorption.
<table>
<thead>
<tr>
<th>Pin ID</th>
<th>Burnup of solid pellet (GW.d/tHM)</th>
<th>Initial Gap Size</th>
<th>Inner radius of annulus (cm)</th>
<th>Plenum Length (cm)</th>
<th>Maximum Clad Hoop Creep Strain</th>
<th>Maximum Rod Internal Pressure (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C8-0217</td>
<td>122.653</td>
<td>1g</td>
<td>0.00</td>
<td>25.40</td>
<td>8.27%</td>
<td>11.03</td>
</tr>
<tr>
<td>C8-0217</td>
<td>122.653</td>
<td>2g</td>
<td>0.00</td>
<td>25.40</td>
<td>6.32%</td>
<td>14.41</td>
</tr>
<tr>
<td>C8-0217</td>
<td>122.653</td>
<td>3g</td>
<td>0.00</td>
<td>25.40</td>
<td>3.89%</td>
<td>19.61</td>
</tr>
<tr>
<td>C8-0217</td>
<td>122.653</td>
<td>4g</td>
<td>0.00</td>
<td>25.40</td>
<td>2.09%</td>
<td>26.00</td>
</tr>
<tr>
<td>C8-0217</td>
<td>122.653</td>
<td>5g</td>
<td>0.00</td>
<td>25.40</td>
<td>0.00%</td>
<td>13.42</td>
</tr>
<tr>
<td>C8-0217</td>
<td>122.653</td>
<td>2g</td>
<td>0.10</td>
<td>25.40</td>
<td>1.97%</td>
<td>12.60</td>
</tr>
<tr>
<td>C8-0217</td>
<td>122.653</td>
<td>2g</td>
<td>0.20</td>
<td>25.40</td>
<td>1.30%</td>
<td>12.35</td>
</tr>
<tr>
<td>C8-0217</td>
<td>122.653</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.82%</td>
<td>12.45</td>
</tr>
<tr>
<td>C8-0413</td>
<td>120.728</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.52%</td>
<td>10.68</td>
</tr>
<tr>
<td>C8-0209</td>
<td>120.567</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.48%</td>
<td>10.58</td>
</tr>
<tr>
<td>D6-0114</td>
<td>114.986</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.37%</td>
<td>9.74</td>
</tr>
<tr>
<td>D6-0114</td>
<td>114.986</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>2.31%</td>
<td>13.82</td>
</tr>
<tr>
<td>D6-1102</td>
<td>114.981</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.34%</td>
<td>9.70</td>
</tr>
<tr>
<td>C8-0516</td>
<td>114.922</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.46%</td>
<td>9.87</td>
</tr>
<tr>
<td>E6-0611</td>
<td>99.956</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.10%</td>
<td>7.84</td>
</tr>
<tr>
<td>E6-0611</td>
<td>99.956</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.34%</td>
<td>10.39</td>
</tr>
<tr>
<td>E6-0611</td>
<td>99.956</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>1.26%</td>
<td>8.70</td>
</tr>
<tr>
<td>C8-1610</td>
<td>99.835</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>2.65%</td>
<td>9.14</td>
</tr>
<tr>
<td>C8-1610</td>
<td>99.835</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.26%</td>
<td>8.17</td>
</tr>
<tr>
<td>D7-0204</td>
<td>99.792</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.39%</td>
<td>9.44</td>
</tr>
<tr>
<td>C8-1111</td>
<td>84.960</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>1.39%</td>
<td>7.74</td>
</tr>
<tr>
<td>C8-1111</td>
<td>84.960</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.18%</td>
<td>7.30</td>
</tr>
<tr>
<td>B8-0817</td>
<td>84.683</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.93%</td>
<td>7.08</td>
</tr>
<tr>
<td>B6-1405</td>
<td>84.592</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.62%</td>
<td>6.96</td>
</tr>
<tr>
<td>B9-0813</td>
<td>59.958</td>
<td>1g</td>
<td>0.00</td>
<td>25.40</td>
<td>1.78%</td>
<td>5.22</td>
</tr>
<tr>
<td>B9-0813</td>
<td>59.958</td>
<td>2.5g</td>
<td>0.00</td>
<td>25.40</td>
<td>0.00%</td>
<td>5.47</td>
</tr>
<tr>
<td>B8-1310</td>
<td>59.900</td>
<td>2.5g</td>
<td>0.00</td>
<td>25.40</td>
<td>0.00%</td>
<td>5.48</td>
</tr>
<tr>
<td>AT-0204</td>
<td>59.501</td>
<td>2.5g</td>
<td>0.00</td>
<td>25.40</td>
<td>0.00%</td>
<td>5.42</td>
</tr>
</tbody>
</table>

Table 3.9: Sample of pins taken from different burnup bins (shaded rows). The Pin ID indicates the location of the fuel pin assessed within the core, with the first two characters referring to the assembly location and the remaining four digits indicating the pin location within an assembly from the bottom left hand corner in terms of row and column location, e.g. 0101 would indicate a fuel pin in the bottom left hand corner and 1717 a fuel pin in the top right hand corner. Burnups displayed are the average across the length of the rod and are from the SIMULATE run containing solid pellets, i.e. as pellet geometry is changed the effect on burnup has not been displayed in this table. The Initial Gap Size corresponds to the pellet-clad gap size at the beginning of life and is shown in terms of a multiple of \( g \), where \( g = 8.2 \times 10^{-3} \) cm (1g is equal to the pellet-clad gap in a typical PWR rod [16]). The Plenum Length is the length of one of the rod’s plenums (there are plenums at the bottom and top of the rod of identical lengths), a larger plenum length will, for a given diameter, result in a larger volume to accommodate fission gases that have been released from the fuel matrix. The maximum clad hoop creep strain is the highest clad hoop creep strain across the entire rod, over the life of the rod. The rod internal pressure and clad hoop creep strain must be below 15.5 MPa and 1% respectively in order to ensure that the likelihood of rod failure is sufficiently low [17].
surpassed 90 GW.d/THM [149]. This is much higher than the peak burnups typically experienced in modern PWRs of around 63 GW.d/THM [16].

Within each of the bins, the fuel rods with the highest burnups were sampled, as the focus was trying to identify the likelihood of rod failure for a given rod geometry, which is more likely at higher burnups. As some assemblies within the core would have burnups with a symmetrical distribution of burnup histories, for example in the central assembly (F06), it is the case that rods in one octant of the assembly will experience the same burnup histories relative to another octant. Therefore, in order to ensure that no rods were effectively analysed twice, rods with identical power histories to previous rods analysed were ignored and another non-identical rod was chosen.

Given the difficulties in currently being able to predict the behaviour of very high gadolinia-doped fuel it was decided to only study the fuel pins that contained no burnable poison. This also seemed appropriate as unsurprisingly the non-BPPs experienced the highest burnups, see Figure B.6, and therefore would be expected to suffer more from the various fuel degradation mechanisms.

To achieve the targeted outlet temperature of 285°C, SIMULATE - which includes a thermal-hydraulics model - predicted an average channel mass flow rate of 57.4 g/s. However, due to the disparity in rod power histories across the core, using 57.4 g/s as the flow rate for all rods resulted in ENIGMA prematurely terminating many runs as ENIGMA predicted that the clad had completely corroded. Hence, initially the coolant flow rate was set to a much higher mass flow rate of 290 g/s per channel to ensure all rods did not fail due to excessive clad surface temperatures. A sensitivity study is later performed in order to assess the dependence of rod behaviour on clad external surface temperature for a variety of rods.

Table 3.9 clearly shows that a pellet-clad gap size of 8.2×10^{-3} cm is insufficient in ensuring that maximum clad hoop creep strains do not surpass 1%, as around 75% of fuel rods in the core have EOL burnups greater than 60 GW.d/THM. However, simply increasing the pellet-clad gap size (thereby accommodating greater pellet swelling at high burnups) increases the amount of fission gas released due to a greater thermal resistance across the larger pellet-clad gap, resulting in a temperature rise in the fuel and excessive fission gas release. To accommodate the higher rod internal pressure due to the extra fission gas release, the plenum volume must be significantly increased by around a factor of 13.

It is possible that due to the very high gadolinia concentrations the thermal conductivity of the BPPs could be severely degraded. This could result in even low burnup BPPs, relative to the highest burnup UO₂ pins, suffering more from degradation (in particular high rod internal pressure and/or high clad hoop creep strain). However, the sparse data on the thermal conductivity of high gadolinia fuel makes it difficult to assess whether this would be true. Hence why work should be performed on gathering data on the thermal conductivity of such fuel.

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13 It is possible that due to the very high gadolinia concentrations the thermal conductivity of the BPPs could be severely degraded. This could result in even low burnup BPPs, relative to the highest burnup UO₂ pins, suffering more from degradation (in particular high rod internal pressure and/or high clad hoop creep strain). However, the sparse data on the thermal conductivity of high gadolinia fuel makes it difficult to assess whether this would be true. Hence why work should be performed on gathering data on the thermal conductivity of such fuel.
two.

Figure 3.26: Peak centreline temperature as a function of time for the highest burnup rod, which was C8-0217, based on two distinct rod geometries. The rod containing solid pellets has an initial pellet-clad gap of 5g, whereas the rod containing annular pellets has an inner radius of 0.20 cm and a pellet-clad gap of 2.5g. Where g = 8.2 \times 10^{-3} \text{ cm}. Note that the rod containing solid pellets will have a significantly higher temperature at the BOL due to the thermal resistance across the very large pellet-clad gap, whereas at the EOL the degradation of thermal conductivity at higher burnups will dominate.

Table 3.9 also shows that it is possible for rods with effectively the same average burnup at the EOL along the length of rods to return significantly different performance parameters; for example, rods E6-0611 and C8-1610 (which are both made up of solid (non-annular) pellets and incorporating a pellet-clad gap of 2.5g) have very different maximum clad hoop creep strain results, see Table 3.9. This was put down to the fact that the two rods have considerably different axial burnup distributions and therefore in the case of rod C8-1610, which had a more skewed distribution, resulted in fuel degradation being heavily concentrated in certain regions of the fuel (see Appendix B.12 for more details).

With respect to the appropriate plenum size, there is likely a preference for shorter plenums in fuel rod design, as a very large plenum of say around 50 cm would probably require an internal support structure which would limit the available volume within the plenum and therefore raise the necessary plenum length to ensure a consistent plenum volume. The larger plenum would perhaps require an increase in the RPV size, which would raise the capital cost of the plant. Therefore it was decided to insist on fuel rods having plenum lengths no greater than 10 inches and seeing what necessary geometry modifications must be made to the pellets in order to achieve this.

Annular pellets are known to show improved swelling behaviour simply because the pellet can swell inwards and therefore this limits the clad hoop stress in comparison to solid (non-annular) pellets [58].
Also by adopting an annular pellet geometry the hottest part of the rod is removed, therefore the average pellet temperature is significantly reduced, limiting thermal expansion and fission gas release. By limiting pellet swelling, which allows a smaller pellet-clad gap to be used and also the removal of the hottest region of the pellet, the peak rod temperature is significantly reduced (see Figure 3.26). The annulus also acts as a volume for fission gas to occupy reducing rod internal pressure for a given plenum volume. In principle annular pellets could allow for the adoption of so-called Dual Cooled Fuel (DCF), where coolant is passed through the centre of the rod. However, to date, there is limited performance data on these rods and therefore they do not fit the requirement that conventional LWR technology is employed. DCF is discussed further in Appendix B.14.

The dual 10 inch plenum length turns out to be an appropriate initial guess; however, the initial gap size is unacceptably small, as the majority of rods in the core do not obey the criteria relating to maximum clad hoop creep strain and rod internal pressure. However, if the gap size were increased from $8.2 \times 10^{-3}$ cm to $2.05 \times 10^{-2}$ cm (resulting in a fuel rod size increase of 2.5% and a reduction in Moderator to Fuel (M/F) ratio of around 5%) the majority of rods would likely survive. In addition, unless some rods incorporate significantly larger plenums then perhaps annular fuel pellets would suffice, although (as is discussed in Section 3.5.4) the reliability of ENIGMA calculations at such high burnups is questionable. Interestingly the Russian VVER-1000 PWR fuel rods have similar pellet-clad gap sizes of $3.0 \times 10^{-2}$ cm, although they utilise thinner pellets in a hexagonal assembly design. VVER rods also employ annular pellets (inner radius of 0.11 cm) [16]; therefore, rods based on VVER-1000 geometries are worthwhile considering in future studies.

Table 3.10 shows the effect of adjusting flow rate on the different rod parameters. There is a general trend for higher temperatures to degrade performance characteristics (due to an increase in internal pressure and an acceleration of clad creep). Table 3.10 also shows that disparity in fuel rod power histories results in a wide range of maximum clad surface temperatures between rods. Unless greater enrichment/poison zoning or an enhanced optimisation process can significantly reduce rod power history disparities, then a logical solution is to insist on variable channel flow across the core in order to minimise the differences in peak coolant temperatures shown in Table 3.10. Otherwise there would be an incredibly large thermal-hydraulic penalty if only a small fraction of the rods are outputting sufficient heat to ensure an adequate temperature rise takes place across the core in addition to the clad degradation that would occur on the hottest rods. Variable channel flow is currently implemented both in BWRs and in some PWRs (of the VVER variety) through the use of zirconium-alloy boxes.
Table 3.10: Dependence of fuel performance properties on channel flow rate for a sample of fuel rods taken from Table 3.9.

<table>
<thead>
<tr>
<th>Pin ID</th>
<th>Flow (g/s)</th>
<th>Maximum Clad Hoop Creep Strain</th>
<th>Rod Internal Pressure (MPa)</th>
<th>Peak Clad Temperature (°C)</th>
<th>Peak Coolant Temperature (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C8-0217</td>
<td>290</td>
<td>0.82%</td>
<td>12.45</td>
<td>287.7</td>
<td>271.2</td>
</tr>
<tr>
<td>C8-0217</td>
<td>200</td>
<td>0.85%</td>
<td>12.62</td>
<td>300.6</td>
<td>278.2</td>
</tr>
<tr>
<td>C8-0217</td>
<td>150</td>
<td>0.93%</td>
<td>12.81</td>
<td>315.5</td>
<td>285.7</td>
</tr>
<tr>
<td>D6-0114</td>
<td>290</td>
<td>0.37%</td>
<td>9.74</td>
<td>287.5</td>
<td>270.0</td>
</tr>
<tr>
<td>D6-0114</td>
<td>150</td>
<td>0.37%</td>
<td>10.00</td>
<td>313.8</td>
<td>283.6</td>
</tr>
<tr>
<td>E6-0611</td>
<td>290</td>
<td>0.34%</td>
<td>10.39</td>
<td>285.7</td>
<td>268.9</td>
</tr>
<tr>
<td>E6-0611</td>
<td>150</td>
<td>0.33%</td>
<td>10.54</td>
<td>309.0</td>
<td>281.5</td>
</tr>
<tr>
<td>D7-0204</td>
<td>290</td>
<td>0.39%</td>
<td>9.44</td>
<td>282.5</td>
<td>268.4</td>
</tr>
<tr>
<td>D7-0204</td>
<td>150</td>
<td>0.36%</td>
<td>9.57</td>
<td>302.7</td>
<td>280.6</td>
</tr>
<tr>
<td>A7-0204</td>
<td>150</td>
<td>0.00%</td>
<td>5.48</td>
<td>283.3</td>
<td>269.9</td>
</tr>
<tr>
<td>A7-0204</td>
<td>100</td>
<td>0.00%</td>
<td>5.54</td>
<td>294.3</td>
<td>277.1</td>
</tr>
<tr>
<td>A7-0204</td>
<td>75</td>
<td>0.00%</td>
<td>5.60</td>
<td>304.8</td>
<td>284.2</td>
</tr>
<tr>
<td>A7-0204</td>
<td>50</td>
<td>0.00%</td>
<td>5.72</td>
<td>324.9</td>
<td>298.0</td>
</tr>
</tbody>
</table>

that surround the sides of the assembly (to stop cross-flow between assemblies) and through the incorporation of artificial blockages to vary channel flow rates between assemblies [150]. Assemblies of this type are referred to as channel boxes or shrouded assemblies. Note that the clad hoop creep strain for variations of pin A7-0204 shown in Table 3.10 is 0.00%, simply because gap closure does not occur until later in life and therefore creep strains are all negative. Hence, the maximum clad hoop creep strain is that at the beginning of life which is 0.00%.

A further peculiar attribute shown in Table 3.10 is that in some of the rods sampled (for example D7-0204) as the rod surface temperature is increased, via reducing the channel coolant mass flow rate, the clad hoop creep strain is reduced. Normally increased temperature increases creep, and the discrepancy in creep between low and high flow rates was too large to be simply attributable to a numerical artefact. The reason behind this unusual behaviour was due to the relatively large gap sizes at the BOL. This results in an acceleration in the initial inwards clad creep (as the pellet-clad gap closes) that was never fully recovered as the creep direction changes. The direction of creep changes as pellets swell as they burnup and this dominates clad hoop strain (see Appendix B.15 for further details).

Table 3.9 indicates that a robust rod design based on a larger gap size of $2.05 \times 10^{-2}$ cm and that contains an inner radius of 0.20 cm would appear to ensure no rod goes beyond the fuel performance criteria specified. It appears likely that all UO$_2$ rods above 100 GW.d/tHM would be required to
adopt this robust rod design, i.e. around 20% of UO$_2$ pins. The vast majority of UO$_2$ pins below 100 GW.d/tHM should be able to adopt the solid (non-annular) pellet geometry but many would likely be required to employ a larger initial gap size from the initial guess size. The neutronic effect of adopting the solid pellet design with a slightly increased pellet-clad gap size of $2.05 \times 10^{-2}$ cm is expected to be small given that the volume ratio of fuel to water is increased by 4.8% when insisting upon a larger gap size, and therefore smaller water volume. Hence, the enrichment limit should not surpass the 20 wt.% given the average rod enrichment is currently around 13.5 wt.%.

3.5.2 Pellet Clad Interaction

Besides the other performance limiting phenomena discussed previously, Pellet Clad Interaction (PCI) is another phenomenon that can lead to the failure of the clad. PCI is a failure mechanism that arises when a fuel rod experiences a rise in power. This rise in power can lead to the pellet imposing high amounts of stress on the clad and chemically aggressive fission products attacking the clad material. As cladding failures during power changes are generally PCI related, and given the relatively frequent power changes the rods will experience in this core, it clearly requires investigation [151].

The mechanical interaction is dominated by the different thermal expansion rate of the Zr-based cladding and UO$_2$ pellets [126]. However, it is unlikely that mechanical interaction alone would result in clad failure [152]. It is the combination of this mechanical stress and the fact that some of the chemically aggressive fission products preferentially attack grain boundaries, thus reducing the stress required for cracks to occur. Furthermore, there is some variation of the susceptibility of rods to experience PCI as burnup increases. This is probably due to the larger inventory of chemically aggressive fission products and greater extent of clad embrittlement (from hydriding, irradiation damage, etc.) [153].

Historically PCI has been more of an issue for BWR fuel rods rather than their PWR counterparts, although PWR rods ramped in test reactors have been shown to be susceptible to PCI induced clad failure. Given this known susceptibility, restricted power ascension rates during PWR startup have been put in place [151, 154].

BWRs have been particularly susceptible to PCI failure as they rely heavily on control blades for reactivity control and the blades have a strong localised flux suppression effect [153]. This suppression can result in sections of fuel having low burnup relative to neighbouring fuel and hence when the blades are withdrawn, a large reactivity and associated power increase can occur. This results in
large localised stress concentrations due to differential thermal expansion rates of the fuel stack and clad. Therefore BWRs have experimented with barriers between the fuel pellet stack and the cladding that reduce the stress applied to the clad [153, 154]. A zirconium-tin alloy which is naturally soft, chemically compatible with the Zr-based cladding and UO$_2$ pellets, in addition to having a low thermal neutron absorption cross-section, has been shown to be an effective barrier in BWR fuel rods [153, 155]. ENIGMA is unable to model this so-called barrier cladding, but it is worth factoring into future studies in order to assess the benefits of such a clad type.

ENIGMA incorporates a PCI model to determine the susceptibility of fuel rods to PCI induced failure. Many of the mechanical interactions are modelled explicitly, such as pellet thermal expansion and the differential movement of pellet segments. However, given the complexity and uncertainty surrounding the chemical mechanisms, they are predominately modelled by weighting factors dependent on the inventory of chemically aggressive fission products and time of exposure to these agents.

The rod with the highest burnup (C8-0217) at the end of core life was exposed to a series of power ramps at yearly intervals from 0 to 15 years inclusive, in order to analyse its susceptibility to PCI failure. The rod had an adjusted geometry based on the data in Tables 3.9 and 3.10, i.e. the mass flow rate was set to 200g/s, the pellet had an inner annulus of 0.20 cm and the pellet-clad gap was $2.5 \times 10^{-3}$ cm. The power ramp studied was from 25% to 100%. Given that the CASMO-SIMULATE model is depleted at 93.5% capacity factor, the rod’s power history was adjusted at certain time steps along its life by multiplying the power level by 0.267 and 1.07 ($0.267 \times 93.5\% = 25\%$ and $1.07 \times 93.5\% = 100\%).
The series of power ramps was based on how this study assumed a container ship powered by a marine reactor would likely operate (see Section 2.4 in the previous chapter for further details). The purpose of this investigation was to find what effect the ramp time period ($t_R$) had on the susceptibility of the fuel to undergo PCI failure. Therefore, the ramp consisted of an initial increase in power from the nominal power output ($P_N = 93.5\%$) to full power ($P_F = 100\%$) over $t_R$, where

$$t_R = \{1s, 1m, 1h\}. \quad (3.8)$$

Three values were used in order to study the sensitivity to the ramp rate. Any dependence of fuel performance to ramp rate is important as this would imply a threshold ramp rate would be necessitated to ensure that the likelihood of PCI failure is low. This threshold would limit the ability of the ship to increase/decrease reactor power as it left/entered port, thereby placing restrictions on the ship’s acceleration/deceleration. Although if the time taken to reach maximum speed was determined to be too long, then an auxiliary diesel engine or a battery could be utilised. This auxiliary engine could be turned off once the reactor had safely reached its maximum power output without the onset of PCI failure.

Once the initial ramp had occurred, the adjustment to power output shown in Figure 3.27 took place over the following time steps ($t_S$)

$$t_S = t_{h1}, t_R, t_{h2}, t_R \quad (3.9)$$

where

$$t_{h1} = 3 \text{ weeks} - t_R \quad (3.10)$$

and

$$t_{h2} = 2 \text{ days} - t_R. \quad (3.11)$$

The series of power ramps shown in Equations 3.10 and 3.11 was repeated three times and the fuel rod was then returned to its nominal power (as outlined in Figure 3.27).

ENIGMA predicted that no fuel failure would occur in the rod exposed to the series of power ramps during its life due to the PCI phenomenon even when utilising a ramp period ($t_R$) equal to 1 s. It is highly unlikely that a fuel rod would be able to sustain a power ramp of 25% to 100% over the course
of 1 s due to the large localised stress occurring within a highly degraded clad (from high burnup) due to differential expansion, and this therefore highlights deficiencies in ENIGMA’s ability to model PCI for the fuel rods in this reactor design. The dearth of data surrounding ultra-high burnup fuel, and therefore the non-existent studies on their PCI performance, implies a large experimental undertaking would be required in order to firstly assess whether rods could survive ramping at high burnups and, assuming survival, create prescriptive ramp limits for operators to follow as ships leave port.

Current data on high burnup rods does not appear to extend much beyond 63 GW.d/tHM [152]. However, it is known that rods at these burnups can survive quite large power ramps without failure, with conditioning powers around 27 kW/m\textsuperscript{14} and a final linear rating of around 40 kW/m\textsuperscript{15}, which is far beyond the highest linear ratings rods experienced in the core designed in this study (see Appendix B.13). It would not be possible to ensure peak burnups below 63 GW.d/tHM in this current core geometry as the average core burnup is considerably above this level. Therefore, either experimental work should be undertaken to calculate prescriptive limits or the number of rods should be increased to significantly reduce peak rod burnup. It is worth noting, however, that current data [152] suggests that the likelihood of rod failure at around 60 GW.d/tHM is approximately the same as the likelihood of rod failure at 40 GW.d/tHM. Therefore whilst the data is spare above around 63 GW.d/tHM, it does not suggest that ultra-high burnup rods are considerably more likely to fail than fuel rods with burnups at around 60 GW.d/tHM.

### 3.5.3 Fatigue

Another phenomenon related to power ramping is fatigue. Most fuel performance codes, including ENIGMA, rely on the fatigue curves produced in Ref. [156] which relate the stress amplitude and/or number of cycles to fuel failure. However, these experiments are based on zircaloy tube bending experiments performed on a variety of fuel rod types which are at best a crude proxy to the bi-axial stresses experienced by fuel rods during power changes throughout their lives, due to radial pellet expansion and axial stress variation. It therefore seemed sensible to look at the typical thermal cycling rods experience in operating conventional reactors.

Normally reactors operate at fairly constant power levels throughout their fuel cycles. Fortunately,

\textsuperscript{14} Conditioning power is based on the pre-ramp power time period being sufficiently long that the pellet-clad gap has closed and the hoop stress is approximately constant, i.e. exhibits little to no time dependence.

\textsuperscript{15} The term linear rating reflects the linear heat density (kW/m) which is typically used to describe the heat generated per unit length of a fuel rod.
the large deployment of nuclear reactors in France necessitates significant power changes throughout their lives in order to match demand for electrical power. Typically a French reactor will undergo around 60 power cycles, of around 100% to 50% and back to 100%, per fuel cycle. Each fuel cycle usually lasts around 12 to 15 months and each rod normally resides within the reactor for 3 fuel cycles (3 to 4.5 years) [157]. Hence, a rod will normally experience around 180 large power cycles throughout its life. It is assumed that in marine core design power cycles occur over a 23 day period (3 weeks at full power, followed by around 2 days in port at partial (25%) power). Hence over its 15 year fuel cycle, the fuel will experience a comparable number of cycles (around 240 large power ramps vs 180 in French fuel rods).

When assessing the likelihood of failure due to fatigue, the magnitude of stress applied during each ramp is of primary importance. The largest component of the stress amplitude (that arises during power cycles) is expansion/swelling of the fuel pellets. Expansion/swelling is primarily determined by the rod operating temperature during the power cycle. This implies that low fuel rod linear ratings are beneficial in limiting the stress amplitude. This is because lower linear ratings imply smaller absolute changes in fuel temperature. French reactors typically have a linear rating of around 17 kW/m, and usually undergo power variations between 8.5 and 17 kW/m [16]. In the core designed in this study, the highest burnup rod has an average rating of around 11 kW/m and experiences typical variations of around 2.8 to 11 kW/m, hence implying that the fuel rods in the reactor designed in this study have favourable characteristics in limiting fatigue failure.

Ideally a comparison would be carried out comparing the fuel rods in the marine reactor with those in French commercial reactors to determine the stress amplitudes in both cases during power ramps. And knowing that fuel rods in French reactors survive a large number of power ramps over their lives, this can be used to assess the likelihood of fatigue failure arising in the fuel rods in the marine reactor. This should be factored into future work.

Finally, the above analysis also suggests that if a marine reactor were to operate under identical power variations of normal cargo ships (with large power variations around once per week, whilst spending around half a dozen hours in port), there will be an increase in the number of cycles from around 240 to around 750 [82]. This is far outside the envelope of experience regarding the total number of cycles rods can withstand. This is a further reason as to why a marine reactor, operating on a 15 year fuel cycle, would likely, at least initially, operate on something similar to a 23 day cycle period.
3.5.4 Validity of ENIGMA at Very High Burnups

Figure 3.28 shows the burnup profile of the rod (pin C8-0217) with the highest burnup and the equivalent burnup profile for the annular version (0.20 cm inner radius). The average burnups across the length of these rods are approximately 120 GW.d/tHM and 150 GW.d/tHM for the solid and annular versions of the fuel rod respectively. These burnups are significantly higher than the burnups fuel rods have been exposed to in LWR conditions.

ENIGMA has been validated up to rod burnups of around 100 GW.d/tHM using data from the Halden Reactor - a 20 MWth Heavy Boiling Water Reactor [158, 159]. This brings into question its ability to accurately model such ultra-high burnup rods, given the nonexistence of validation data at such high burnup levels.
Figure 3.29: SEM radial scan of a fuel sample at 73 GW.d/tHM that exhibits High Burnup Structure (HBS)[32]. The pellet outer (cooler) region is on the right of the image and shows the transition between the restructured HBS region (on the right) and the effectively intact microstructure around 100 µm from the outer surface.

Probably the greatest uncertainty relating to modelling fuel rods at ultra-high burnups is the formation of so-called High Burnup Structure (HBS). At low temperatures (less than around 1100°C) the fuel undergoes a restructuring process at around 50 GW.d/tHM which results in a new morphology referred to as HBS, see Figure 3.29. HBS is characterised by many small grains and a large number of small pores containing fission gases. Hence HBS exhibits a much higher amount of porosity relative to the rest of the fuel pellet.

HBS forms due to resonant neutron capture in $^{238}\text{U}$, which causes a build up of $^{239}\text{Pu}$ in the peripheral region of the fuel pellet. The increase in fissile $^{239}\text{Pu}$ leads to an increase in burnup relative to the average pellet burnup by a factor of around 2.5 [160]. The extent of HBS along the pellet radius increases from the outer surface with higher burnup, and therefore gradually more and more of the pellet transforms into HBS. Whilst there is no clear consensus on the exact mechanism for the restructuring process some beneficial fuel performance characteristics are observed, these are [160]:

- In the HBS region, fission gas retention is very high$^{16}$.
- The restructured region shows an increase in softness.
- The restructuring process appears to remove defects from the lattice, thereby reducing phonon scattering events, and improving thermal conductivity.

HBS also exhibits the following detrimental characteristics [160]:

$^{16}$ Whilst fission gas retention is high in the HBS region, it is still the case that fission gas release increases as a function of burnup. The main reason for this discrepancy between localised and overall fission gas release is believed to be due to the increase in centreline temperature as a function of burnup [160].
• The increase in porosity reduces the beneficial impacts on thermal conductivity associated with recrystallisation. This is because the pores are occupied by fission gases that exhibit very low thermal conductivity.

• The swelling that results from the porosity formation will increase the stress applied to the clad material.

The overall effect on thermal conductivity is a slower reduction in this property than would otherwise likely occur if restructuring did not take place. This is because the restructuring process counteracts to a some extent the accumulation of defects in the lattice associated with, for example, a build up of fission products. The restructuring process also offsets the increase in porosity attributable to HBS formation. Hence, under normal operating conditions, the formation of HBS is probably beneficial with respect to fuel performance. However, under off-normal (accident) conditions, such as reactivity insertion accidents due to a rod ejection, or a loss-of-coolant accident, then the formation of HBS can result in the following sequence of events [161, 162]:

• The fission gas bubbles in the HBS region are heated up and expand.

• This expansion can cause the fuel to fragment as large internal forces are generated within the pellet.

• During the off-normal event, the increased rod temperature can also cause the clad to expand (balloon).

• The fragmented fuel can then more easily relocate within a rod as it expands. For instance fragmented fuel in the top of the rod can fall to the bottom portion of the rod.

• Any buildup of fuel within a region can concentrate the amount of heat generated within that location. This can result in further clad expansion within this region and eventual clad failure.

• As the fuel is fragmented it can readily be ejected from the rod once rupture has occurred.

Hence, HBS formation can not only increase the likelihood of clad failure during certain accident scenarios but can result in a fuel form that can be more readily dispersed, resulting in highly active fuel entering the coolant. Therefore, HBS formation is a considerable disadvantage in off-normal operating conditions.
Any uncertainty into the extent and response of fuel performance to HBS is clearly important in being able to confidently predict the behaviour of the fuel rod. The current ENIGMA model performs the following calculations regarding the formation and behaviour of HBS:

- ENIGMA employs empirical correlations (on data from experiments up to around 100 GW.d/tHM) to predict the extent of HBS formation.
- The porosity is then calculated within this region based on empirical data.
- The effect porosity formation has on thermal conductivity and swelling are calculated.

ENIGMA cannot currently factor in that HBS has not been observed at temperatures above around 1100°C, and therefore can predict unphysical phenomena relating to HBS formation at high fuel temperatures. This is probably less of a concern with annular pellets, where peak pellet temperatures are approximately below this temperature limit and thus it is possible that certain pellets within the rod are made up of entirely HBS (see Figure 3.28).

Recent evidence has shown a small but significant improvement in the thermal conductivity behaviour of small pellet samples of highly irradiated fuel that have developed HBS, relative to irradiated disks that have not developed HBS due to operating significantly above the 1100°C temperature limit [160]. There is in general a decrease in the thermal conductivity as a function of burnup, due to the accumulation of defects in the crystal lattice (from fission product impurities, cracks, bubbles, radiation damage, etc.). These defects impact phonon scattering processes and thus decrease thermal conductivity (see Section 4.6.1 in Chapter 4 for more details on this phenomenon).

The increase in thermal conductivity as HBS forms has been attributed to the restructuring mechanism reducing defects in the HBS region, and thus reducing phonon scattering mechanisms and therefore improving the material’s thermal conductivity. Over time the small increase in thermal conductivity is reduced as burnup increases and further accumulation of damage offsets the benefit of the HBS restructuring process. Therefore, the net effect of HBS formation is a slower degradation of thermal conductivity relative to a pellet where no HBS has formed.

In general the HBS region only penetrates a relatively small distance into the pellet width (typically less than around 100 µm) and therefore the net benefit is usually small. However, in the case where effectively the entire pellet could consist of High Burnup Structure, then the benefit would be expected to be more pronounced - as is the case for pellets in certain rods within the core being studied here.
The heavy dependence of fuel performance on the extent of HBS and the current uncertainty regarding the extent of the characteristics associated with high burnup structure formation imply that it would be worthwhile to perform a sensitivity study on the various effects of HBS formation (such as porosity) and overall fuel performance. ENIGMA currently does not incorporate any freedom for the user to vary the various parameters the High Burnup Structure routine impacts and hence does not allow the user to perform sensitivity analysis. It is suggested to incorporate this into future work.

Given the sparseness of experimental data on the performance of LWR fuel rods above around 100 GW.d/tHM it is suggested that future work targets limiting maximum rod burnups to below 100 GW.d/tHM.

3.6 Summary

This investigation has shown that the optimised marine core has exhibited the following neutronic characteristics:

- Robust against the various effects of xenon;
- Obeys the criteria put in place concerning Rod Ejection Accidents (at the cost of increasing the number of Rod Control Cluster Assemblies (RCCAs) to 81);
- Exhibits acceptable MTC and Doppler coefficients throughout life;
- Achieves the necessitated shutdown margins (although at the expense of increasing the number of RCCAs from 81 to 89).

However, issues relating to the ability of CASMO-SIMULATE to model a hardened-spectrum core have arisen, due to the necessary high enrichment required to meet the targeted core life. Nevertheless, many of the neutronic criteria put in place, for example the shutdown margin, were easily surpassed when insisting every assembly has an RCCA; the uncertainty was not large enough to render the results meaningless as the underlying physical phenomena predicted are likely to be correct, for example the behaviour of the core to xenon transients.

However, the fuel rod geometry used in the core design has been shown to be inappropriate from a fuel performance perspective and therefore future work should include rods with an overall
diameter around 2.5% greater than the current rod versions in order to accommodate pellet swelling. In addition, the disparity in rod power histories across the core suggests either one, or a mixture of the following, is performed in future work:

- A more complex, automated optimisation routine is put in place (see the Conclusion chapter for further details);
- Minimise peaking factors throughout life to reduce the divergence in maximum clad surface temperature and rod End of Life (EOL) burnups;
- The limitation on identical rod geometries throughout the core is removed;
- Investigate the benefit of channel boxes (shrouded assemblies).

This shrouded assembly strategy, whilst perfectly viable and well demonstrated in operating LWRs, should ideally be limited to a certain number of assemblies in order to minimise the parasitic absorption of neutrons by excess material in the core (as the boxes surrounding the assemblies result in excess material within the neutron field and will adversely impact the neutron economy). It may be the case that variable rod geometries could alone suffice in minimising the divergence in maximum clad surface temperatures for a given flow rate and/or only certain assemblies require channel boxes.

Until data on higher burnups is available, it appears sensible to minimise peak burnup to less than 100 GW.d/tHM. This is simply because rods at these high burnups have been shown to obey the various fuel performance criteria, such as fission gas release, fuel swelling and the ability of the clad to survive these ultra-high burnups [39]. In addition, future work should incorporate experimental measurements of the thermal conductivity of high gadolinia content pellets (in excess of 20 wt.%) at a variety of temperatures, to extend the current database on high gadolinia fuel and allow the performance of high gadolinia fuels to be studied in detail.

It would also be beneficial for ENIGMA to allow the user to perform sensitivity analyses on the various parameters the High Burnup Structure routine varies such as the extent of porosity, as well as allowing the user to include recent data showing a slowdown in the degradation of thermal conductivity as the high burnup structure develops.

A major issue relating to fuel performance is the dearth of data relating to the Pellet Clad Interaction (PCI) performance of rods exposed to burnups is excess of around 63 GW.d/tHM and this creates an issue regarding the ability to confidently predict the behaviour of rods during ramping at
burnups in excess of 90 GW.d/tHM. To a lesser extent fatigue is also an issue but data on fuel rods in French reactors - that experience a large number of repeated power ramps throughout their life - could be used to assess the ability of zirconium-based fuel rods to experience a series of cyclic stresses.

Finally, from a neutronics perspective, benchmarking of various thermal lattice codes to hardened-spectrum cores is required and should be performed.
Chapter 4

Thorium Core

4.1 Outline

The incorporation of ThO$_2$ into a core capable of achieving the design parameters set out in Chapter 2 was performed. This was to assess the merits of such a fuel mixture in the low power density core design in this study. The neutronic characteristics of the resulting core were studied and compared to those of the UO$_2$ core. There have been limited studies on the suitability of multi-group data libraries used in deterministic reactor physics codes for modelling thorium-uranium oxide ((Th,U)O$_2$) fuelled cores and therefore a comparison was made with the continuous BINGO nuclear data library in MONK and the 70 group library in CASMO 4.

To date there have also been very limited fuel performance studies comparing precisely what attributes of (Th,U)O$_2$ makes this fuel type superior or inferior to UO$_2$ fuel. Whilst it is known that ThO$_2$ exhibits some favourable properties including lower fission gas release and significantly improved thermal conductivity [163], there has been very little work assessing how these and other fuel performance properties behave as a function of U content. This is probably due to insufficient data on the many fuel properties that are required in order to accurately determine the behaviour of a fuel type. These properties include: thermal conductivity, diffusion coefficients, creep rates, thermal expansion coefficients and elastic moduli. Therefore an assessment was performed on two of the most important properties in oxide fuel [126]: thermal conductivity and diffusion coefficients.

ENIGMA currently attempts to model the behaviour of (Th,U)O$_2$ fuel; however, it assumes that
many of the properties are similar to UO$_2$ fuel due to insufficient data to disprove this assumption. The suitability of ENIGMA’s current database on thermal conductivity and fission gas release was investigated and the performance of the fuel rods in the (Th,U)O$_2$ core were assessed.

4.2 Motivations

The primary interest in utilising (Th,U)O$_2$ fuel for the reactor being investigated in this study was to assess its behaviour as a fertile poison. Unlike burnable poisons (where a neutron is absorbed and then the absorbing nuclide transmutes into a nuclide with a very low absorption cross-section), a fertile poison absorbs the neutron and then will transmute into a fissile nuclide. This assumes any intermediate nuclides do not drastically interfere with the efficiency of this process. The production of fissile material is beneficial to neutron economy.

Other secondary motivations included:

- Reduced neutronic penalties associated with the fission products of $^{233}$U relative to $^{235}$U, due to lower fission product yields for the most parasitic neutron absorbers. In particular the precursor nuclide to $^{135}$Xe, which is $^{135}$I, has a lower yield (4.9% vs 5.6%) which should make xenon transients more benign [89].

- Given the low power density of the core designed in this study, this should limit the destruction of the intermediate nuclides (see Section 4.3.2), allowing the core to minimise the loss of $^{233}$U.

- It is generally stated [164, 18, 165] that (Th,U)O$_2$ fuel has advantageous physical properties which should result in its fuel performance being better than that of UO$_2$ fuel.

4.3 The Thorium Fuel Cycle

In this section the benefits of the open and closed thorium-uranium (Th-U) cycle relative to the equivalent uranium-plutonium (U-Pu) cycles are discussed. The focus is on solid oxide fuels as this is the form of fuel being deployed here, and there is a far greater wealth of data to analyse the relative performance of the different aspects of the fuel cycles, namely: neutronic characteristics, fuel behaviour, fuel manufacture, proliferation resistance, reprocessing and waste disposal. It is worth
noting that when analysing fuel cycles based on alternative fuel forms to those of oxide fuels the analysis becomes far more subjective due to the limited data available.

4.3.1 Overview of the Thorium Fuel Cycle

Thorium (Th) effectively exists in nature as only one isotope (\(^{232}\text{Th}\)) which is fertile and therefore analogous to \(^{238}\text{U}\). For conciseness, \(^{232}\text{Th}\) will be referred to as thorium. In the presence of a neutron flux thorium will undergo the reactions (with the half-lives shown)

\[
^{232}\text{Th} + n \rightarrow ^{233}\text{Th} \quad 22.3 \text{ min} \rightarrow ^{233}\text{Pa} \quad 27.0 \text{ days} \rightarrow ^{233}\text{U},
\]

thereby producing fissile \(^{233}\text{U}\).

For comparison the set of fertile-to-fissile nuclear reactions for \(^{238}\text{U}\) are shown

\[
^{238}\text{U} + n \rightarrow ^{239}\text{U} \quad 23.5 \text{ min} \rightarrow ^{239}\text{Np} \quad 2.35 \text{ days} \rightarrow ^{239}\text{Pu},
\]

Thorium is around three times more abundant than uranium in the earth’s crust [18]. However, fast neutron reactors are able to exploit uranium reserves via the U-Pu cycle such that they could produce enough global primary energy to last for millennia [18]. Therefore, assuming fast reactors can achieve commercial maturity, the scarcity of uranium is only important in the very long term. Hence, the abundance of thorium is more relevant to countries that are concerned with their energy security and have large deposits of thorium, but relatively few uranium deposits (as is the case in India [52]).

4.3.2 Neutronic Characteristics

Perhaps the single greatest benefit of the thorium-uranium fuel cycle is the neutronic characteristics of \(^{233}\text{U}\). \(^{233}\text{U}\), as shown in Table 4.1, has a very high \(\eta\) value. This value represents the number of neutrons released on average per neutron absorbed, and in order to achieve a conversion ratio greater than 1, \(\eta\) must be above 2.0. Of the nuclides listed Table 4.1 it is only practical to breed \(^{239}\text{Pu}\) and \(^{233}\text{U}\). In fact of these two nuclides only \(^{233}\text{U}\) exhibits an \(\eta\) value greater than 2.0 at all neutron energies in a reactor [165]. However, at fast neutron energies \(^{239}\text{Pu}\) has a superior \(\eta\) value (2.8 vs 2.5 for \(^{239}\text{Pu}\) and \(^{233}\text{U}\) respectively) and therefore is able to achieve much higher conversion ratios in fast reactors.
Table 4.1: Neutronic parameters of key nuclides [18, 19]. Absorption has been defined here as the sum of radiative capture and fission cross-sections, with cross-sections based on neutrons travelling at 2200 m.s\(^{-1}\). \(\eta\) is prompt critical reactivity margin and \(\eta_{th}\) is the average number of neutrons released per thermal neutron absorbed.

Since \(\eta_{th}\) is above 2.0 this permits a fuel cycle based on Th-U to become self-sustaining in technically mature thermal reactors but, as will be discussed in this chapter, many other areas of the Th-U cycle are much less technically mature. Other neutronic benefits include the higher thermal absorption cross-section of thorium compared to \(^{238}\)U, see Table 4.1, which aids in the conversion of thorium to \(^{233}\)U.

Acting against these benefits is the relatively long half-life of the precursor nuclide to \(^{233}\)U: \(^{233}\)Pa. Any destruction of \(^{233}\)Pa - via neutron bombardment - before it becomes fissile \(^{233}\)U adversely affects the neutron economy. Hence, from a neutronics perspective, it is favourable to deploy Th-based fuel in reactors with low neutron fluxes and therefore low power densities.

An alternative option would be to remove the \(^{233}\)Pa from the high flux region of the core and then reintroduce it into the core once it has decayed to \(^{233}\)U. The latter approach is employed in liquid fuelled reactor concepts such as some designs of the Molten Salt Reactor (MSR). This explains the interest in deploying MSRs utilising the Th-U fuel cycle. However, most experience regarding MSRs comes from the Molten Salt Reactor Experiment (MSRE). This was a very small (7.5 MW(th)) reactor that operated intermittently over a 5 year period until 1969 [165]. It would require a large R&D effort to scale this up to a commercial scale plant able to reliably output hundreds of mega-watts for time periods measured in decades.

## 4.3.3 Fuel Behaviour

The behaviour of (Th,U)\(\text{O}_2\) fuel is complicated by the fact that many of its performance characteristics depend heavily upon the concentration of U in the (Th,U)\(\text{O}_2\) fuel. Furthermore, the temperature the
fuel operates under can lead to \((\text{Th, U})\text{O}_2\) fuel performance being better or worse than \(\text{UO}_2\) fuel at the same temperature. Hence, it is not possible to say in general terms whether the overall characteristics of Th-based fuel are superior or inferior to those of \(\text{UO}_2\) fuel. Section 4.6 discusses in detail how key performance phenomena (namely fission gas release and thermal conductivity) behave as a function of temperature and U content.

There are some general characteristics that hold true independent of the temperature regime or uranium content. These are [34]:

- Creep is generally lower in \((\text{Th, U})\text{O}_2\) fuel. This is disadvantageous as low creep rates tend to limit the ability of the fuel to deform under an applied stress. The deformation will usually result in a reduction in stress, through a process known as stress relaxation.

- The lower density of \(\text{ThO}_2\) fuel \((10.0 \text{ g.cm}^{-3})\) compared to \(\text{UO}_2\) fuel \((10.96 \text{ g.cm}^{-3})\) implies that for the same power output \((\text{Th, U})\text{O}_2\) fuel will achieve a higher burnup than the equivalent \(\text{UO}_2\) fuel. This is unfavourable because performance characteristics tend to degrade as burnup increases.

- The melting point is higher for \((\text{Th, U})\text{O}_2\) fuels. However, this has only a relatively small benefit over \(\text{UO}_2\) fuel as this latter oxide’s melting point \((2800^\circ \text{C})\) is also very high.

There is some concern [163] relating to thorium’s limited number of oxidation states relative to uranium. This is because once fission has occurred, the liberated oxygen atoms from \((\text{Th, U})\text{O}_2\) fuel will have fewer elements within the fuel to combine with relative to \(\text{UO}_2\) fuel. It is likely that any liberated oxygen atoms will combine with one of the following: fission products from the lanthanoid series (as they typically have a large number of oxidation states); any uranium present in the fuel or zirconium in the clad material. If the latter occurs then this will result in the internal corrosion of the clad, thereby increasing the likelihood of fuel failure for a given thickness of clad material. Data from the Shippingport [163] experiments did not find any major issues regarding the internal oxidation of the Zr-alloy clad; however, their burnups were relatively low in comparison to the core being studied here \((< 60 \text{ GW.d}/\text{tHM}) [163]\). If it is the case that future experimental work shows internal oxidation of the clad to be excessive, then one option to reduce the likelihood of liberated oxygen from reacting with the internal clad walls would be to introduce an oxygen ‘getter’ to the \((\text{Th, U})\text{O}_2\) pellets.
4.3.4 Manufacturing Fresh (Un-Reprocessed) Fuel

The fabrication of (Th,U)O$_2$ fuel is similar to that of UO$_2$, with comparable sintering times and temperatures between the two fuel types [163, 33, 166]. Furthermore, the reported achievable fuel densities, as a percentage of theoretical density, are also comparable [33].

India has manufactured Th-based oxide fuels in large quantities (tens of tonnes) [164]. Therefore there are no major technical barriers with respect to the manufacturability of (Th,U)O$_2$ fuels nor any considerable detrimental cost implications. Hence, with respect to fuel manufacturing it believed that the performance of (Th,U)O$_2$ vs UO$_2$ fuel are broadly similar.

4.3.5 Proliferation Resistance

Firstly, it should be stated that all nuclear fuel cycles entail some proliferation risks as the ability to release large quantities of energy from a small amount of matter is inherently useful for both peaceful and non-peaceful purposes. Nevertheless, the light water reactor once-though cycle does not directly create any weapons usable material and has become the benchmark for non-proliferation [52]. Furthermore, it is important to distinguish between a ‘nuclear weapon’ and a ‘nuclear device’. Here, a nuclear weapon is considered a system that is capable of creating an assured yield and is deliverable over long distances, i.e. it has a high military value. A nuclear device on the other hand does not have to be mountable on a modern delivery system nor have a high reliability in producing the intended yield. States would have the greatest interest in developing nuclear weapons, whereas non-state groups may be content with a nuclear device [167].

This leads to a key point regarding proliferation resistance: technologically there is little that can be done to stop a determined state from obtaining nuclear weapons. For this reason this discussion will focus on non-state actors.

Advantages regarding the proliferation resistance of the Th-based fuels include:

- Penetrating gamma radiation, due to the co-production of $^{232}$U, makes detecting diverted material easier.
• Dilution (denaturing) of fissile $^{233}$U is possible with $^{238}$U\textsuperscript{1}.

• Chemically separating thorium from $^{233}$U is more complex.

The disadvantages include:

• The bare sphere critical mass for $^{233}$U is relatively low (around 15 kg compared with around 10 kg and 50 kg for $^{239}$Pu and $^{235}$U respectively) [164].

• The spontaneous fission rate is much lower than for $^{239}$Pu which permits $^{233}$U to be implemented in a much simpler weapons design (a so-called ‘gun-type’ design) [164].

$^{232}$U is produced via a variety of (n,2n) reactions during irradiation of Th/$^{233}$U fuel (for example $^{233}$U(n,2n)$^{232}$U), and whilst some of the decay products of $^{232}$U are strong gamma emitters (for example $^{208}$Tl), these highly active species are not sufficient to stop determined individuals (whom we assume give less regard for their well-being) from constructing a nuclear device [167, 169]. Furthermore, experiments carried out on $^{233}$U have utilised the fact that separating out some of the elements necessary to build up sufficient quantities of highly penetrating gamma-emitting nuclides, results in relatively low doses from $^{232}$U contaminated fuel [35, 36]. It would subsequently take around 7 days for a significant inventory of highly penetrating nuclides to emerge, which may be sufficient time to construct a crude device without being exposed to a lethal radiation dose [164]. However, as stated above, the presence of a highly penetrating form of radiation aids in detecting diverted materials.

With respect to denaturing, Forsberg and Hopper [170] proposed that in order to ensure that sufficient denaturing for mixtures of $^{233}$U, $^{235}$U and $^{238}$U has occurred, that the following formula, referred to here as the Proliferation Index, should be obeyed:

$$\frac{\text{Weight of } ^{233}\text{U} + 0.6 \times \text{Weight of } ^{235}\text{U}}{\text{Total uranium weight}} < 0.12 \quad (4.3)$$

This is based on the fact that the critical mass for a metal sphere of uranium containing 12 wt.% $^{233}$U is approximately the same as the critical mass for a metal sphere of uranium containing 20 wt.% $^{235}$U [170].

\textsuperscript{1}It would be possible to separate out the denatured $^{233}$U from $^{238}$U. However, this would necessitate access to enrichment technology and if non-state actors were to have access to such systems then a major non-proliferation barrier would have already been removed. Furthermore, the addition of $^{238}$U into the fuel before irradiation will inevitably result in significant quantities of $^{239}$Pu; however, this already occurs in spent nuclear fuel from conventional LWRs. In addition, the plutonium quality will be somewhat lower, as a larger concentration of the heat-emitting $^{238}$Pu will be produced when thorium is present [132, 168].
In assessing the proliferation resistance of the closed Th-U cycle we have placed limited weight on physical barriers (such as fences, alarms, guard forces, etc.) and much more weight on intrinsic properties of the separated $^{233}\text{U}$, with realistic impurity levels of $^{232}\text{U}$ and its associated daughter products [171]. The reasoning behind this approach is that physical barriers may not have as high a degree of reliability as the intrinsic barriers, namely the material properties of the separated fissile medium (critical mass, heat generation, associated radiation field and neutron emission rate) [171].

In conclusion, assuming separation has not been carried out and sufficient denaturing has occurred then the proliferation resistance of $^{233}\text{U}$ is deemed to be broadly similar to that of Spent Nuclear Fuel (SNF) from conventional LEU fuelled reactors. On the other hand, if separation has occurred which results in relatively pure $^{233}\text{U}$, i.e., some contamination with $^{232}\text{U}$, no denaturing, and virtually no fission products/minor actinides present, then the proliferation resistance becomes unfavourable relative to the equivalent U-Pu cycle. This is because in such a scenario there are fewer technical barriers to creating a nuclear device once $^{233}\text{U}$ has been obtained. However, it is best to avoid any reprocessing cycle that creates such streams, be it Pu or $^{233}\text{U}$, and this is in fact one of the drivers for advanced reprocessing cycles [52]. Finally, it may be possible to incorporate an additive during fresh fuel manufacturing that will increase the inventory of $^{232}\text{U}$ in the spent fuel. This would, however, further increase shielding requirements for manufacturing pellets from reprocessed fuel and would very unlikely be sufficient to incapacitate someone quickly enough such that they are unable to construct a nuclear device [169].

4.3.6 Reprocessing

Reprocessing spent UO$_2$ fuel is carried out in the commercially mature PUREX cycle. The most developed process for reprocessing thorium oxide fuel is the so-called THOREX cycle, which is a modification of the PUREX process [164]. There are a large number of similarities between the THOREX and PUREX cycles; however, as the chemical stability of thorium oxide is very high, this significantly complicates the dissolution phase in the THOREX cycle. In particular, (Th,U)O$_2$ fuel exhibits low solubility in the hot nitric acid solution used to dissolve conventional UO$_2$ spent fuel [165]. Therefore a catalyst, in the form of hydrofluoric acid, is added in order to accelerate the dissolution process. However, excess fluoride ions can corrode the vessels that the process is carried out within and hence aluminium nitrate is added to remove the fluoride ions that do not partake in fuel dissolution [165].
Any aluminium nitrate that passes through the plant will become part of the fission product inventory, thereby increasing the volume of waste that needs to be vitrified. The volume increase is around 50% relative to the conventional PUREX process for an equivalent amount of spent UO₂ fuel. Furthermore, any fluoride compounds that enter the vitrification plant could create corrosion issues given the extremely high operating temperatures of these plants.

There is also the added complexity associated with then manufacturing the reprocessed (Th,U)O₂ fuel as the decay products of any ²³²U present result in having to increase the shielding requirements relative to manufacturing conventional mixed oxide (MOX) fuel [164]. As was stated in the previous section, it is possible to chemically separate out elements that eventually decay to highly active gamma emitters, although this would weaken one of the proliferation benefits associated with the Th-U cycle.

It appears to be the case that historical experience with the THOREX cycle was at the pre-industrial scale, with around 200 tonnes of (Th,U)O₂ being reprocessed via this method [172, 173]. Therefore, it is certainly not the case that the THOREX cycle is very immature but its added complexity, larger volumes of vitrified waste and the uncertainty regarding scalability imply it has significant drawbacks relative to the PUREX cycle. Hence, the reprocessing performance of (Th,U)O₂ fuel is deemed unfavourable relative to spent UO₂ fuel.

4.3.7 Waste Disposal

The radiotoxicity of spent fuel from a closed or open Th-U fuel cycle is in general lower than in conventional U-Pu cycles [18]. However, in the case of a closed cycle the radiotoxicity is considerably lower due to fact there would be far fewer transuranics [165]. Radiotoxicity as a metric for the performance of spent fuel in a repository is, however, limited. This is because the minor actinides are relatively immobile under repository conditions [167] and therefore these components of nuclear waste should be relatively well isolated from humans and the environment over periods of time measured in tens of millennia.

Far more important is the heat output from the nuclear waste, as there is concern that if the thermal energy is sufficiently high it could degrade the host geology [167]. From this respect an open Th-LEU cycle is broadly similar to an open U-Pu cycle [164]. A closed Th-U cycle may have a lower heat output since the transuranics contribute significantly to the outputted thermal energy, although the difference in fission product yields may counteract these benefits - there is limited information in the public domain regarding this attribute of closed Th-U cycles.
A significant benefit from a waste disposal perspective of (Th,U)O$_2$ fuel relative to UO$_2$ fuel is the chemical stability of (Th,U)O$_2$. Whilst the low solubility of (Th,U)O$_2$ is problematic with respect to reprocessing it does imply that as a host matrix for containing geologically mobile radionuclides it is preferable to UO$_2$ [174]. Hence, overall an open Th-U cycle is advantageous relative to an open U-Pu cycle with respect to waste disposal. However, it appears that a closed Th-U fuel cycle is broadly similar to the closed U-Pu cycle from a waste disposal perspective. Although if it is shown that the heat generation of the closed Th-U cycle is considerably higher or lower than a closed U-Pu cycle, then this would be sufficient to deem the waste disposal performance unfavourable or favourable respectively.

4.3.8 Summary of the Performance of the Thorium-Uranium Cycle

<table>
<thead>
<tr>
<th>Process</th>
<th>Favourable</th>
<th>Broadly Similar</th>
<th>Unfavourable</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proliferation Resistance</td>
<td>■</td>
<td>✔</td>
<td>●</td>
</tr>
<tr>
<td>Manufacturing Fresh Fuel</td>
<td>●</td>
<td>■</td>
<td>✔</td>
</tr>
<tr>
<td>Reprocessing</td>
<td>✔</td>
<td>■</td>
<td>●</td>
</tr>
<tr>
<td>Waste Disposal</td>
<td>■</td>
<td>✔</td>
<td>●</td>
</tr>
</tbody>
</table>

Table 4.2: Evaluation of the performance of open and closed Th-U cycles relative to their U-Pu counterparts. The green square indicates the performance of the open Th-U cycle and blue dot indicates the performance of the closed Th-U cycle. By definition, no reprocessing takes place in the open Th-U cycle and therefore its relative performance is not shown. Due to lack of publicly available data, it has been assumed that the heat generation from reprocessed (Th,U)O$_2$ fuel is broadly similar to that of reprocessed (U,Pu)O$_2$ fuel. If heat generation turns out to be significantly lower or higher, then the blue dot would move to either favourable or unfavourable respectively.

The benefits of the Th-U fuel cycle relative to the U-Pu cycle depend upon whether it is implemented in an open or closed cycle. Furthermore, there is the complication from a neutronics perspective at least that it is preferable to deploy U-Pu in fast reactors, whereas the neutronic characteristics of thermal and epithermal reactor systems favour Th-U fuels. In addition, fuel performance is highly dependent on the operating conditions of the reactor and is discussed in detail throughout this chapter. A summary of the evaluation of the remaining areas of the Th-U fuel cycle is shown in Table 4.2, with blue dots representing the closed Th-U cycle and green squares representing the open Th-U cycle.

It should be noted that when commercial entities (such as utility companies) make decisions with respect to implementing a new fuel type the importance of the different factors in Table 4.2 will not
all be equal. For instance, the economic costs for disposing of nuclear waste per unit of spent fuel are relatively low and therefore even if the characteristics of the waste from the new fuel type are superior, this will have little direct impact on the overall costs associated with the new fuel type.

The remainder of this chapter focuses on implementing an open cycle thorium-LEU reactor design since this avoids many of the detrimental impacts associated with closed Th-U cycles.

4.4 Neutronics of (Th,U)O₂ Core

4.4.1 Optimisation

A very similar process was performed to that in the previous chapter for choosing the lattice contents: enrichment, burnable poison concentrations and number of Burnable Poison Pins (BPPs), radial and axial enrichment and poison distribution throughout the core. The main difference from the procedure described in the previous chapter was the complication of having an extra variable to modify: the relative concentration of thorium to uranium. In order to simplify matters it was decided to set the ²³⁵U content in any uranium present in the reactor to 19.5 wt.% to ensure that the boundary between LEU and HEU was of no concern and the proliferation index was below 0.12 at the beginning of life. Therefore the enrichment was effectively adjusted by altering the relative concentration of thorium to uranium in the fuel rods; this had the desired effect of altering the concentration of fissile material within the fuel rods. It also meant that the largest practical amount of thorium was introduced to the core in order to assess what benefits thorium addition to the core would have on its behaviour over time.

Choosing Lattice Contents

Whilst thorium’s thermal neutron capture cross-section is significantly larger than ²³⁸U (7.4 b vs 2.7 b) it is not possible in the reactor being considered in this investigation to operate the core without utilising Burnable Poison (BP) to minimise the reactivity swing. This is because the absorption cross-section is too small to satisfactorily suppress k_{eff} at beginning of life using thorium alone (for comparison gadolinium has a thermal absorption cross-section of 4900 b).

Once again the burnable poison gadolinium was employed although it must be stressed that the data necessary to accurately predict fuel performance as a function of burnup for gadolinium-doped
thoria/urania fuel appears to be non-existent and the same appears true for any appropriate BP that could be used with (Th,U)O$_2$ fuel$^2$.

Figure 4.1: $k_\infty$ evolution as a function of thorium content for an infinite array of 17 by 17 assemblies. Thorium content is shown as a weight percent of total heavy metal content.

Figure 4.1 shows how altering the concentration of thorium to uranium in fuel rods (with no BP present) affects reactivity over core life. It was therefore appropriate to investigate (Th,U)O$_2$ fuel that incorporated < 50 wt.% thorium into the fuel, otherwise the thorium displaces too much fissile bearing U and does not permit the 15 year core life to be achieved.

As was the case in the previous chapter a series of colourset models were constructed to screen potential combinations of lattice configurations. The criteria relating to number of distinct lattice configurations, relative concentration of the burnable poison Gd$_2$O$_3$, and enrichment/fissile content, were the same as in the previous chapter. Figure 4.2 shows the chosen lattice configuration that was subsequently implemented into SIMULATE.

$^2$Technically the use of ZrB$_2$ as a layer applied to the surface of the fuel pellets is advantageous with respect to fuel performance modelling as it does not directly influence the thermal conductivity of the pellets. Therefore unpoisoned fuel data can be used as ZrB$_2$ is not mixed into the fuel material. However, as discussed in the Section 2.8 of Chapter 2, the BP boron is inappropriate for the reactor being studied in this investigation.
Figure 4.2: Result from coloursset model (2D solution) for a lattice combination of alternating 96 Burnable Poison Pin (BPP) lattices and 76 BPP lattices. The 76 BPP lattice had a thorium content of 30 wt.% and the BPPs contained 10.5 wt.% Gd\(_2\)O\(_3\). The 96 BPP lattice had a thorium content of 27.5 wt.% and the BPPs contained 9.5 wt.% Gd\(_2\)O\(_3\).

The criteria in place when constructing finite cores in SIMULATE were:

1. The \(k_{\text{eff}}\) at the Beginning of Life (BOL) was chosen to be approximately 1.0;

2. At the End of Life (EOL) \(k_{\text{eff}}\) must be greater than or equal to 1.0.

In the previous chapter the initial \(k_{\text{eff}}\) criterion for the UO\(_2\) core was slightly higher as it was assumed that around 1000 pcm would be required to compensate for xenon transients. However, the UO\(_2\) core analysis found that due to the low power density it was insensitive to xenon transients. Hence, it was decided to relax this criterion.

As was the case in the UO\(_2\) core, it was found that employing a ratio of around two 96 BPP lattices to one 76 BPP lattice resulted in reactivity profiles that met the \(k_{\text{eff}}\) criteria at BOL and EOL.

**Radial Optimisation of Core Layout**

Figure 4.3 shows the initial guess at the core layout and final chosen core layout, with Table 4.3 showing the contents of the assemblies in Figure 4.3. The chosen radial distribution criteria were the same as for the UO\(_2\) core, namely that at the start of life the power should be highest in the central region of the core and also have a relative power fraction in this region of less than around 1.5. Figure 4.4 shows the improvement in radial power distribution between the initial guess at an appropriate
loading pattern and the final chosen loading pattern once shuffling and replacement of assemblies had taken place.

Figure 4.3: Radial optimisation with respect to core layout was based on an initial guess for an appropriate core layout, Profile 1. The assemblies were then shuffled and, where necessary, swapped until a desired power profile was achieved, which was that the relative power fraction in the central region of the core, at the start of life, should be highest and be \( \leq 1.5 \). Profile 2 shows the core layout that achieves the desired power profile. The colours and numbers represent assembly IDs with their contents shown in Table 4.3.

Figure 4.4: Radial power profiles for core layouts shown in Figures 4.3a and 4.3b at \( t = 0 \). The radial power profile is taken from a slice through the central assembly and includes the assembly with the highest relative power fraction. In the case of Profile 1, this was a diagonal slice through the core and includes assembly D8, which was where the power was the highest. Profile 2 on the other hand is a radial slice through row 6 of Figure 4.3b as the power peaked in assembly F6 for this core at the beginning of life. Profile 1 refers to the initial guess at core layout and Profile 2 shows the final chosen core layout.
<table>
<thead>
<tr>
<th>Assembly ID</th>
<th>Th to Th+U (wt.%%)</th>
<th>Gd(_2)O(_3) content (wt.%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>96</td>
<td>22.5</td>
<td>8.5</td>
</tr>
<tr>
<td>96</td>
<td>27.5</td>
<td>9.5</td>
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<tr>
<td>96</td>
<td>32.5</td>
<td>10.5</td>
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<tr>
<td>76</td>
<td>25</td>
<td>9.5</td>
</tr>
<tr>
<td>76</td>
<td>30</td>
<td>10.5</td>
</tr>
<tr>
<td>76</td>
<td>35</td>
<td>11.5</td>
</tr>
</tbody>
</table>

Table 4.3: Breakdown of individual assembly contents. The assembly IDs correspond to those in Figure 4.3b, with the number in the assembly ID describing the number of BPPs within that assembly.

Figure 4.5: \(k_{\text{eff}}\) evolution for the radially optimised core.

Figure 4.5 shows the \(k_{\text{eff}}\) evolution for the radially optimised core. Due to the lower \(k_{\text{eff}}\) criterion at the beginning of life for the (Th,U)O\(_2\) core relative to the UO\(_2\) core, the (Th,U)O\(_2\) core in its current form was incapable of maintaining \(k_{\text{eff}} \geq 1.0\). However, it was assumed this would be addressed in the axial optimisation process as the rules set out in the axial optimisation process specified that the final core layout must be capable of maintaining criticality throughout its life (see below).

**Axial Poison and Enrichment Optimisation**

Starting with the core layout shown in Figure 4.3b the core was divided (as before) into three regions: a top Low Poison (LP) region, a middle High Poison (HP) region and a bottom LP region. The chosen Rod Control Cluster Assembly (RCCA) configuration was the same 81 RCCA configuration from the previous chapter (see Figure 3.10b in the previous chapter). The banks were also offset by 10% of core height and the order of bank penetration was kept the same, i.e. bank 1 would enter first and
once it was inserted 10% of the way into the core bank 2 would follow, and so forth.

As was the case for the UO$_2$ core, the bottom axial region was varied over lengths of 1, 5, 10 and 20 cm. However, the top axial region was varied over 70, 80, 90 and 100 cm, whereas previously the top axial regions were varied over 40, 60, 80 and 100 cm. This was because the UO$_2$ discriminator algorithm generally returned cores with a top axial region length in the range 80 to 100 cm. Hence, in order to speed up the process of creating a viable core design it was decided to focus the search space around 80 to 100 cm.

The list of poison variations made to assemblies in Table 4.3 for the core in Figure 4.3b is shown in Table 4.4.

<table>
<thead>
<tr>
<th>Lattice type</th>
<th>Poison variation (wt.%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
</tr>
<tr>
<td>76-HP</td>
<td>6.375</td>
</tr>
<tr>
<td>76-LP</td>
<td>-7.5</td>
</tr>
<tr>
<td>96-HP</td>
<td>-0.375</td>
</tr>
<tr>
<td>96-LP</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 4.4: The variations in poison concentrations made to the lattices with 76 and 96 Burnable Poison Pins (BPPs), divided into High Poison (HP) and Low Poison (LP) regions, made to the assemblies shown in Table 4.3 along with how the poison variations were grouped together (indicated by matching coloured cells).

As was the case for the UO$_2$ core, 4 alterations to the fissile content were made. For the UO$_2$ core these alterations were 0.75, 0.5, 0 and -1 wt.%, which for the (Th,U)O$_2$ core is equivalent to thorium content variations of -3.75, -2.5, 0 and 5 wt.% - recall that increasing the thorium content is the same as decreasing enrichment and the remaining U within the rod has a fixed enrichment of 19.5 wt.%, so a 5 wt.% increase in Th content results in roughly a 1 wt.% decrease in $^{235}$U.

The discriminator algorithm used in the previous chapter was also used to determine the preferred core configuration of the 9216 cores run. However, it returned no core configurations that fulfilled the criteria regarding sufficient reactivity over core life and small control rod penetration ($< 50\%$ of active core height). It was found that the majority of the 9216 cores did not have sufficient reactivity to achieve the chosen core life of 15 years. Therefore the thorium content variations were altered to: -7.5, -5, 0 and 2.5 wt.% which correspond roughly to enrichment variations of 1.5, 1, 0 and -0.5 wt.% respectively.

Rerunning the 9216 cores with the new thorium content variation resulted in around 200 valid core configurations, with the assembly contents for the core with the lowest through-life local peaking factor shown in Table 4.5. The sizes of the bottom and top axial regions were 1 cm and 90 cm.
respectively; therefore in reality the bottom axial region was having negligible effect.

The assembly contents outlined in Table 4.5 shows that assemblies with 76 burnable poison pins have a slightly higher poison content in the Low Poison regions relative to the High Poison regions of the lattices. However, the enrichment is much higher in the Low Poison region and therefore the reactivity in all Low Poison regions within this core is much higher than the corresponding High Poison regions; it would have been more appropriate to call the Low Poison and High Poison regions High Reactivity and Low Reactivity regions respectively.

<table>
<thead>
<tr>
<th>Lattice key</th>
<th>High Thorium content (wt.%)</th>
<th>Low Thorium content (wt.%)</th>
<th>High Poison content (wt.%)</th>
<th>Low Poison content (wt.%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>96</td>
<td>25</td>
<td>15</td>
<td>15.625</td>
<td>5.5</td>
</tr>
<tr>
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<td>30</td>
<td>20</td>
<td>16.625</td>
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</tr>
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<td>35</td>
<td>25</td>
<td>17.625</td>
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</tr>
<tr>
<td>76</td>
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<td>76</td>
<td>32.5</td>
<td>22.5</td>
<td>10.125</td>
<td>10.5</td>
</tr>
<tr>
<td>76</td>
<td>37.5</td>
<td>27.5</td>
<td>11.125</td>
<td>11.5</td>
</tr>
</tbody>
</table>

Table 4.5: Breakdown of individual lattice contents. The lattice IDs correspond to those in Figure 4.3b. The high poison region that contains burnable poison pins and unpoisoned fuel pins will have a high thorium content (low enrichment) level, whereas the low poison region will have a low thorium content (high enrichment) at levels specified above.

In the subsequent sections of this chapter this radially and axially optimised core configuration will be analysed with regards to the depth of control rods, shutdown (sub-criticality) margins, rod ejection accidents, reactivity coefficients, core behaviour with respect to temporal and spatial distribution of xenon and fuel performance.

4.4.2 Control Rod Analysis

Control Rod Heights

Figure 4.6 shows how the RCCAs move throughout core life in terms of mean RCCA insertion and the depth of the deepest RCCA. The deepest RCCA insertion throughout core life was equivalent to 49% of the core height. Also note that after 15 years the deepest RCCA is still penetrating the active core region (around 13%).
Shutdown Margins

The RCCAs consisted of a hafnium tip equal to 49% of core height since in the (Th,U)O\textsubscript{2} core no control rod penetrates more than 49% of the way into the core during power operation. The remaining 51% consisted of boron carbide. Figure 4.7 shows the dependence of $k_{\text{eff}}$ over core life with 81 and 89 RCCAs fully inserted into the core minus the highest-worth rod.

As was the case for the UO\textsubscript{2} core, the 81 RCCA configuration was unable to achieve the necessary shutdown margin of $k_{\text{eff}} < 0.95$ under Cold Zero Power (CZP) conditions with no xenon present.
Increasing the number of RCCAs to 89 resulted in the shutdown margin criteria being met. Under Hot Zero Power (HZP) conditions the required $k_{\text{eff}}$ value of less than 0.98 throughout core life was met with 81 RCCAs, which was also the case for the UO$_2$ core. Therefore the shutdown margin characteristics of the (Th,U)O$_2$ core were broadly similar to those of the UO$_2$ core.

Shutdown cooling calculations were also performed (see Appendix C.1) showing that the maximum reactivity increase was around 1100 pcm, which was similar to the maximum reactivity increase found during shutdown cooling with the UO$_2$ core (around 1000 pcm). In both cores the sub-criticality margin with 89 RCCAs minus the highest-worth RCCA inserted is sufficient to overcome any increase in reactivity due to the change in nuclide inventory as a function of time.

**Rod Ejection Accidents**

As previously, the highest-worth rod throughout core life was ejected for the 81 RCCA configuration and the associated reactivity increase was compared to the reactivity margin between delayed and prompt critical (see Figure 4.8).

![Figure 4.8: Reactivity increase associated with the ejection of the Highest-Worth RCCA (HWR) and the associated 1 dollar margin (along with a ± 10% uncertainty) vs time.](image)

The (Th,U)O$_2$ generally showed improved margins between the reactivity increase associated with the highest-worth RCCA ejection and the prompt criticality in comparison to the UO$_2$ core. This is
unlikely to be due to the characteristics of any $^{233}\text{U}$ fuel present in the core. As Table 4.1 shows, for a thermal spectrum core the beta value for $^{233}\text{U}$ is much less than $^{235}\text{U}$’s beta value. $^{232}\text{Th}$ does possess a much larger beta value than $^{235}\text{U}$ and $^{238}\text{U}$ (see Table 4.1); however, in a thermal/epithermal reactor this benefit is meaningless since the likelihood of thorium fissioning in such a reactor is incredibly small as the fission cross-section for $^{232}\text{Th}$ only becomes significant for neutron energies above 1.4 MeV [18].

Figure 4.9: $k_{\text{eff}}$ evolution for the (Th,U)O$_2$ and UO$_2$ cores without control rods present.

Figure 4.9 shows the $k_{\text{eff}}$ evolution for the (Th,U)O$_2$ and UO$_2$ cores without control rods present. Whilst the removal of control rods results in a core depleting differently to a core with control rods present (hence the reason why both of the un-rodded cores are unable to sustain criticality for the 15 year period) it does allow for estimation of the reactivity increase at certain points in time when rods are removed. It can be seen that towards the beginning of life the (Th,U)O$_2$ core exhibits lower excess reactivity relative to the UO$_2$ core, whereas towards the end of life the opposite is true. Therefore the likely reason for the difference in Rod Ejection Accident behaviour is simply due to the difference in reactivity profiles of the two cores returned by the discriminator algorithm.

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4.4.3 Reactivity Coefficients

Figure 4.10: Variation of Moderator Temperature Coefficient as a function of time and core state. The core states investigated were Cold Zero Power (CZP), Warm Zero Power (WZP), Hot Zero Power (HZP) and Hot Full Power (HFP).

Figure 4.10 shows the dependence of the Moderator Temperature Coefficient (MTC) on core life and coolant temperature. Recall from the previous chapter that Cold Zero Power (CZP), Warm Zero Power (WZP) and Hot Zero Power (HZP) corresponded to coolant temperatures of 20°C, 100°C and 255°C. Hot Full Power (HFP) had an inlet and outlet temperature of 255°C and 285°C respectively.

Figure 4.10 shows that the (Th,U)O$_2$ core generally exhibited more negative MTC values than the equivalent case from the UO$_2$ core (see Figure 3.14 in the previous chapter). This is perhaps because the dependence of the power distribution over time is different between the (Th,U)O$_2$ core design and the equivalent U core. Hence, in the (Th,U)O$_2$ case the thermal neutron population towards the end of life may be focused in a region of the core where there is more $^{235}$U or $^{233}$U and therefore any change in coolant density will have a more pronounced effect on MTC.
Figure 4.11 shows the dependence of Distributed Doppler Coefficient (DDC) on core life and coolant temperature. The DDC is in general slightly less negative than the DDC from the UO$_2$ core (see Figure 3.15 in the previous chapter). This is probably because there is less $^{238}$U in the (Th,U)O$_2$ core relative to the UO$_2$ core and $^{238}$U has a significantly larger resonance integral compared to $^{232}$Th (275 b vs 85 b). Hence, it would be expected that the DDC is weaker in a (Th,U)O$_2$ core relative to the UO$_2$ core.

In general the MTCs and DDCs are comparable and negative throughout life in both the Th-LEU and U cores. However, the HZP cases in the (Th,U)O$_2$ core do not exhibit the reactivity coefficient changes later in core life witnessed in the UO$_2$ core, where in the UO$_2$ case they became significantly less negative. The reason for this is unclear.

### 4.4.4 Power Profiles

The radial and axial power distributions for the radially and axially optimised (Th,U)O$_2$ core are shown along with a discussion regarding any significant differences between this core and the equivalent UO$_2$ core from the previous chapter.
Figure 4.12: Radial power profile as a function of time when the core is depleted with Rod Control Cluster Assemblies present.

The radial power profile from the (Th,U)O$_2$ core is shown in Figure 4.12. The main difference between the radial power profile for this core and the UO$_2$ core is that the UO$_2$ core generally had a radial power profile that peaked in column C, whereas the (Th,U)O$_2$ core’s profile is peaked towards the centre of the core. Furthermore, the UO$_2$ core radial power distribution generally underwent very little radial power redistribution throughout core life, whereas the (Th,U)O$_2$ core undergoes significant radial power change.

Figure 4.13: Power distribution of the rod with the highest burnup at end of life (located in assembly F6) as a function of time.

Figure 4.13 shows the linear rating profile for the rod with the highest burnup (pin F61304) in the (Th,U)O$_2$ core. The peak in the power profile moves from the top half of the rod to the bottom half.
of the rod over a period of around 5 years; for comparison the equivalent rod in the UO\textsubscript{2} core (pin C80217 - see Figure 3.18 in the previous chapter) has its peak linear rating concentrated in the top half of the rod for the first 12.5 years. The peak linear ratings throughout their respective lives are roughly the same (around 33 kW/m and 30 kW/m for the rods from the (Th,U)O\textsubscript{2} core and UO\textsubscript{2} core respectively). Hence, even though the density of the (Th,U)O\textsubscript{2} fuel rods is significantly lower than the UO\textsubscript{2} fuel rods, the peak core burnups are very similar since the power profile for pin F61304 is more evenly spread across the length of the rod in comparison to pin C80217 in the UO\textsubscript{2} core.

This highlights a deficiency in the discriminator algorithm used to determine the most appropriate core configuration, as one of its criteria was to output cores in ascending order of the largest local peaking factors throughout each of the core’s lives that passed the other criteria, without considering the spatial and time dependence of the local peaking factor. For instance, consider the case with two cores that both have the same largest local peaking factor but with distinct spatial and time dependence on the local peaking factor, which are:

- In one core the local peaking factor moves from one region of the core to another throughout core life never returning to a region that has previously experienced the largest local peaking factor.

- In the other core the local peaking factor is concentrated in one region of the core throughout core life.

In the former case the burnup of each region of the core will be similar; however in the latter case the range of burnups will be very large as one region will have a considerably higher burnup relative to the other core regions. It would therefore have been more appropriate to utilise a metric that factors in a preference for low peak rod burnups. However, low local peaking factors are also important as whilst a core may contain rods with low peak rod burnups, this does not factor in the distribution of burnup along the length of the rod, which is also an important characteristic. For instance, if a small section of a rod experiences burnups above 150 GW.d/tHM with the remainder experiencing around 80 GW.d/tHM, this rod is likely to show poorer characteristics than a rod with peak axial region burnups of 100 GW.d/tHM, even if the latter case has a higher average axial burnup. Hence, it would have been better for the discriminator algorithm to return cases where burnups were below a certain threshold and then order these cores by local peaking factor. This is discussed in further detail in the Conclusion.
Finally, the axial offset throughout core life is shown in Figure 4.14. The average axial offset throughout core life for the (Th,U)O₂ core was -0.007, which implies that axial power distribution was relatively symmetrical over the course of core life. For comparison the average axial offset throughout life for the UO₂ core was 0.252.

4.4.5 Burnup Histories

Figure 4.15 shows the range of burnup histories at the end of life for all rods. As was the case for the equivalent histogram for the UO₂ core, the distribution in rod burnups is very large, although a far
greater number of unpoisoned (Th,U)O₂ rods have a burnup in the range 97.5 to 125 GW.d/tHM.

Figure 4.16 displays the axial burnup distribution for the rods with the highest burnup in the UO₂ and (Th,U)O₂ cores. The average rod burnups at the end of life for both rods are around 120 GW.d/tHM.

As was discussed in Section 4.4.4, the integrated power density of each region over the course of pin F61304’s life is more similar than is the case for pin C80217 in the UO₂ core. This explains why the burnups are very similar even though the (Th,U)O₂ has a significantly lower density than the UO₂ rod. However, pin F61304 does have a relatively low burnup in the bottom region of its rod, therefore there is likely scope to further flatten the burnup distribution by making the bottom axial region (currently 1 cm) larger and altering the enrichment/poison concentration in the fuel to compensate for changes in reactivity as the axial region sizes change.

4.4.6 Proliferation Index

SIMULATE does not output to the user the total inventory of ²³³U. Therefore, a CASMO lattice calculation was used to infer whether or not the proliferation index criterion set out in equation 4.3 was likely to be obeyed for the (Th,U)O₂ core. This calculation used a lattice with 76 BPPs containing 15 wt.% Gd₂O₃ and a thorium content of 35 wt.% as a percentage of total heavy metal content, which was representative of the lattices within the optimised (Th,U)O₂ core. All remaining
pins also contained 35 wt.% thorium. Figure 4.17 shows how the proliferation index varies as a function of time and is always below the 0.12 limit required by Equation 4.3.

![Proliferation Index vs Time Graph](image)

Figure 4.17: Proliferation index as a function of time for a lattice containing 76 BPPs with a thorium content of 35 wt.% and a poison concentration of 15 wt.% Gd$_2$O$_3$.

### 4.4.7 Xenon Fission Product Effects

#### Xenon Transients

<table>
<thead>
<tr>
<th>Time transient initiated</th>
<th>Peak Xe time</th>
<th>Associated reactivity decrement</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 d</td>
<td>1.4 h</td>
<td>-5 pcm</td>
</tr>
<tr>
<td>5.0 y</td>
<td>2 h</td>
<td>-2 pcm</td>
</tr>
<tr>
<td>10.0 y</td>
<td>2 h</td>
<td>-2 pcm</td>
</tr>
<tr>
<td>15.0 y</td>
<td>1.8 h</td>
<td>-13 pcm</td>
</tr>
</tbody>
</table>

Table 4.6: Details the negative reactivity insertion associated with xenon transients taking place at various points in core life under Hot Zero Power conditions.

Table 4.6 shows the negative reactivity insertion associated with xenon transients taking place at various points in core life for the (Th,U)O$_2$ core which were in general smaller than those for the UO$_2$ core. The (Th,U)O$_2$ core was able to overcome all xenon transients from conditions of Hot Zero Power.
at peak xenon and return the core to Hot Full Power. The improved xenon transient behaviour relative to the UO$_2$ core design was attributed to the fact that the control rods have a deeper penetration towards the EOL in the Th/LEU core and therefore have greater reactivity margins to overcome xenon transients. Furthermore, the flux is generally harder throughout life in the (Th,U)O$_2$ core compared to the UO$_2$ core (see Figure 4.18) and, as was discussed in Section 4.3.2, the poisoning effects of fission products, in particular iodine/xenon, are weaker.

![Figure 4.18: Comparison of thermal fluxes throughout core life for the (Th,U)O$_2$ and UO$_2$ cores.](image)

Given the relative insensitivity of the core (Th,U)O$_2$ core to xenon it was assumed that the core would also be insensitive to radial and axial xenon oscillations as was the UO$_2$ core. Therefore radial and axial xenon oscillations were not studied.

### 4.5 MONK Analysis

A comparison was made between MONK using the BINGO JEF 2.2 continuous nuclear data library and the 70 group JEF 2.2 nuclear data library employed in CASMO. As was the case for the UO$_2$ core, three cases were run representing 3 distinct lattice types with some having similarities to those found in the (Th,U)O$_2$ core. All cases had fuel temperature equal to the moderator temperature which was 528 K and contained an infinite array of 17 by 17 lattices with rod geometries identical to those found in the (Th,U)O$_2$ core designed in this study. The three cases modelled were:

1A) (Th,U)O$_2$ fuel pins containing 80 wt.% Th as a percentage of the heavy metal content, with the remaining 20 wt.% consisting of uranium enriched to 19.5 wt.% $^{235}$U.

2A) (Th,U)O$_2$ fuel pins containing 27.5 wt.% Th as a percentage of the heavy metal content, with
the remaining 72.5 wt.% consisting of uranium enriched to 19.5 wt.% $^{235}$U.

3A) $(\text{Th},\text{U})_2\text{O}_3$ fuel and burnable poison pins containing 27.5 wt.% Th as a percentage of the heavy metal content, with the remaining 72.5 wt.% consisting of uranium enriched to 19.5 wt.% $^{235}$U. There were 96 BPPs and these contained 16.5 wt.% Gd$_2$O$_3$, with the remainder of the fuel containing a $(\text{Th},\text{U})_2\text{O}_3$ mixture identical to the fuel pins present in the rest of the lattice.

<table>
<thead>
<tr>
<th>Case</th>
<th>$(\text{Th},\text{U})_2\text{O}_3$ Discrepancy</th>
<th>UO$_2$ Discrepancy</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$k_{\text{fast}}/k_{\text{total}}$ (%)</td>
<td>$k_{\text{fast}}/k_{\text{total}}$ (%)</td>
</tr>
<tr>
<td>1A</td>
<td>0.199</td>
<td>0.966 ± 0.021</td>
</tr>
<tr>
<td>2A</td>
<td>0.436</td>
<td>1.21 ± 0.14</td>
</tr>
<tr>
<td>3A</td>
<td>0.577</td>
<td>1.49 ± 0.02</td>
</tr>
</tbody>
</table>

Table 4.7: Assessing discrepancy as a function of spectrum type (using the metric $k_{\text{fast}}/k_{\text{total}}$) for $(\text{Th},\text{U})_2\text{O}_3$ and UO$_2$ lattices. The discrepancy is between CASMO using a JEF 2.2 70 group nuclear data library and MONK using the JEF 2.2 BINGO continuous data library.

Table 4.7 shows the difference in discrepancy between Cases 1A to 3A for the $(\text{Th},\text{U})_2\text{O}_3$ lattices and Cases 1A to 3A from the UO$_2$ lattices in the previous chapter. The results show that the discrepancy is significantly higher for the $(\text{Th},\text{U})_2\text{O}_3$ lattices in comparison to the similar UO$_2$ lattices. In fact, even though Case 1A of the $(\text{Th},\text{U})_2\text{O}_3$ variant has a significantly softer spectrum in comparison to the equivalent UO$_2$ variant the discrepancy is much higher. The likely reason for the higher discrepancies for the $(\text{Th},\text{U})_2\text{O}_3$ lattices is due to the 70 energy group structure employed by CASMO-4 being optimised for $^{235}$U and $^{238}$U lattices with limited enrichment and poison concentration. Therefore, certain resonances in $^{232}$Th are inadequately modelled, thus resulting in the higher discrepancy between the continuous and 70 energy group structures.

4.6 Fuel Performance

4.6.1 Thermal Conductivity

Of all the various properties that determine the performance of oxide fuel, probably the most important is the behaviour of thermal conductivity, simply because many degradation mechanisms exhibit strong temperature dependence and the thermal conductivity of oxide fuel is very low [126, 33].

In UO$_2$ and $(\text{Th},\text{U})_2\text{O}_3$ pellets the conduction of heat occurs via phonons and/or the kinetic energy
of electrons. Therefore the thermal conductivity can be expressed as:

\[ \lambda = \lambda_{ph} + \lambda_{el} \]  

(4.4)

where \( \lambda_{ph} \) and \( \lambda_{el} \) represent the phonon and electronic contributions to thermal conductivity respectively. In ThO\(_2\) fuel (where no uranium is present) there is no \( \lambda_{el} \) contribution due to the difference in electronic band structure in ThO\(_2\) fuel relative to UO\(_2\) fuel [163, 175]. ENIGMA assumes that for all thorium-based fuels \( \lambda_{el} \) is zero which is likely a relatively poor assumption for thorium-based fuels with high concentrations of uranium. For fuels with an electronic contribution then at temperatures below 1500 K the phonon contribution dominates and as the temperature increases beyond this limit the electronic contribution becomes more pronounced [126]. As oxide fuel temperatures are usually below approximately 1500 K the missing \( \lambda_{el} \) contribution for (Th,U)O\(_2\) fuel is of limited concern and therefore only the phonon contribution is discussed in detail here.

From empirical studies and theoretical models it has been shown that the phonon contribution can be represented as [126]

\[ \lambda_{ph} = \frac{1}{A + BT} \]  

(4.5)

where \( A \) corresponds to the scattering of phonons by imperfections in the lattice structure that are independent of temperature (such as fission gas bubbles or the addition of metal ions) and \( B \) corresponds to temperature dependent phonon-phonon scattering interactions. ENIGMA currently assumes that the \( A \) term for (Th,U)O\(_2\) fuel increases linearly with burnup (as is the case in UO\(_2\) fuel) due to the fact that the buildup of fission products in the lattice acts as phonon scattering sites thereby degrading thermal conductivity. Given that no data is available to determine the behaviour of \( A \) as a function of burnup for (Th,U)O\(_2\) fuel ENIGMA assumes that the increase in \( A \) is identical to that for UO\(_2\) fuel.

It appears that most work measuring the thermal conductivity of (Th,U)O\(_2\) fuel has focused on relatively small U additions of less than 30 wt.%., i.e. the pellets have been predominantly Th [163]. The most extensive dataset found in terms of temperatures, and U to Th concentrations, was the Korean dataset in Ref. [33]. Figure 4.19 also includes the values of thermal conductivity predicted by the models employed in ENIGMA.

ENIGMA originally implemented the Belle and Berman (B&B) model [34] for determining the thermal conductivity of Th-based oxide fuel up to 30 wt.%.. Extrapolating the B&B model beyond
Figure 4.19: Thermal conductivity for 95% dense (Th,U)O$_2$ and UO$_2$ as a function of temperature and, in the case of (Th,U)O$_2$ fuel, as a function of U concentration. Data is shown from the experimental results in the Korean dataset in Ref. [33]. Belle and Berman (B&B) [34] devised a correlation for calculating the thermal conductivity of (Th,U)O$_2$ fuel up to U fractions of 30%. The B&B correlation was modified in order to extend the range of applicable U concentrations and give reasonable agreement with the Korean dataset and ENIGMA’s current correlation for calculating the thermal conductivity for UO$_2$ fuel.

30 wt.% is inappropriate as it results in non-physical negative thermal conductivities and gives very poor agreement with the empirical data found on U concentrations in (Th,U)O$_2$ fuel above 30 wt.%.

Therefore, using the Korean dataset and the existing B&B model, in addition to ENIGMA’s well validated model for calculating the thermal conductivity of pure UO$_2$ fuel, it was decided to construct a simple modified B&B model. The modified B&B model consists of taking the value of thermal conductivity from the B&B model at 30 wt.% U and then using this value for the remaining concentrations. This appeared to give reasonable agreement with the datasets shown in Figure 4.19. As more data becomes available the modified B&B model devised in this study can be updated in future work.

Figure 4.19 also illustrates how the different datasets diverge depending on the temperature range. This can be explained in terms of phonon scattering whereby the $A$ term in Equation 4.5 becomes more dominant as the temperature decreases. Phonon scattering results from the imperfections in the lattice structure and therefore at low temperatures the measured $\lambda_{ph}$ will become more dependent on the microstructure of the prepared fuel sample. Furthermore, thermal conductivity measurements are
usually carried out on small samples and therefore any distribution in porosity, which would effectively be isotropic on the scale of a pellet, also becomes more significant. In addition, for both the B&B and more recent Korean datasets, the experimental uncertainties are not discussed, therefore making it difficult to carry out a detailed comparison. Nevertheless, given the limited data, the modified B&B appears an appropriate model to utilise for determining the thermal conductivity of (Th,U)O$_2$ fuel. It also highlights deficiencies in the published (Th,U)O$_2$ data that should be targeted in future work.

Figure 4.19 shows that whilst ThO$_2$ exhibits improved thermal conductivity, as the U concentration increases the thermal conductivity quickly approaches that of UO$_2$ and the Korean dataset shows that at certain concentrations (around 60 wt.% U) the thermal conductivity is below that of UO$_2$. It is believed [163] that the observed general depression of thermal conductivity in (Th,U)O$_2$ fuels is due to the mixture of heavy metal ions that act as phonon scattering centres and therefore impact term $A$ in Equation 4.5.

The above thermal conductivity degradation behaviour is important as whilst it is usually stated that ThO$_2$ exhibits superior thermal conductivity behaviour to UO$_2$ [164, 18, 165] (which is true when factoring in the sensitivity of fuel performance to even small changes in thermal conductivity) in reality, however, one is only interested in cases where Th has been mixed with some concentration of U (or Pu). This is because a pure thorium oxide rod would not contribute any significant power for a very large proportion of its life without some fissile content present. Only in the case of breeder blankets would pure thorium oxide material be of use; however, even in this case breeder blankets typically contribute very little to overall core power [176].

4.6.2 Fission Gas Release

As was discussed in the previous chapter, ensuring that the rod internal pressure is below the external pressure of the coolant is an important performance criterion when assessing the behaviour of fuel rods. This rod internal pressure is primarily determined by the extent that gaseous fission products (predominantly Xe and Kr due to their high fission yields and low solubility limits) have escaped the fuel matrix.

An important mechanism in determining the extent of Fission Gas Release (FGR) is how individual gas atoms migrate through the fuel pellet. On the scale of a crystal lattice it appears to be the case that the diffusion of single gas atoms is governed by the behaviour of vacancies [177]. This can be

---

A similar behaviour has been observed in (U,Pu)O$_2$ mixtures and (Th,Pu)O$_2$ mixtures [163].
attributed to the fact that for diffusion to occur the fission gas atom must acquire enough energy for it to jump from one lattice position to another. Hence, the single gas atom diffusion coefficient \((D)\) is utilised. \(D\) is made up of the three components [126]

\[
D = D_{th} + D_{\text{mix}} + D_{\text{ath}} \tag{4.6}
\]

where for UO\(_2\) fuel

\[
D_{th} = 1.14 \times 10^{-8}\exp\left(-\frac{35000}{T}\right), \tag{4.7}
\]

\[
D_{\text{mix}} = 1.5 \times 10^{-17}\exp\left(-\frac{10600}{T}\right)\sqrt{q}, \tag{4.8}
\]

\[
D_{\text{ath}} = 6 \times 10^{-23}q \tag{4.9}
\]

with \(q\) being the rating in kW/kgHM and \(T\) is the absolute temperature. The three components of \(D\) are used to describe the three distinct temperature regimes that the single gas atom diffusion coefficient depends on [126]. At temperatures above \(\sim 1400\) K a purely thermally-activated diffusion process appears to dominate. This thermally-activated process corresponds to thermally created vacancies and corresponds to \(D_{th}\). At temperatures below approximately \(1000\) K a so-called irradiation-enhanced diffusion process dominates corresponding to \(D_{\text{ath}}\). This athermal process arises as the fission fragments and their associated irradiation damage cascades interact with the fission gas atoms in the lattice, resulting in the displacement of the gas atoms. In the region \(1000-1400\) K, vacancies necessary for gas atom diffusion are assumed to be created by both thermal and damage cascades, which is described by term \(D_{\text{mix}}\). In conventional LWRs it is the \(D_{\text{mix}}\) component that dominates.

Figure 4.20 depicts the behaviour of each of these components as functions of temperature with a rating \((q)\) equal to \(14\) kW/kgHM (representative of the average rating for fuel rods within the core being studied here).
Most of the work relating to the diffusion of gaseous and volatile fission products in thorium-based fuels has been performed with: low uranium concentration (< 10 wt.%); low burnups (much less than 40-50 GW.d/THM burnups in conventional LWRs); and temperatures above 1400 K [178]. The very limited set of experiments have shown that the release of the gaseous and volatile species has been an order of magnitude lower than in UO$_2$ fuel. Therefore the available experimental data supports altering the thermally activated diffusion coefficient ($D_{th}$). Hence, ENIGMA only alters this component in the single gas atom diffusion coefficient ($D$) with $D_{th} = 1.14 \times 10^{-9} \exp\left(-\frac{35000}{T}\right)$ for (Th,U)O$_2$ fuel, where $T$ is the absolute temperature.

There are a number of key fuel performance areas in ENIGMA that currently assume that the behaviour of (Th,U)O$_2$ fuel is identical to that of UO$_2$, for instance the models used for determining High Burnup Structure formation and Pellet Clad Interaction in UO$_2$ fuel are used in an unaltered state for modelling the same processes in (Th,U)O$_2$ fuel. This is simply because no data are available to contradict these assumptions.

### 4.6.3 Behaviour of Sampled Rods from (Th,U)O$_2$ Core

The same process described in the previous chapter was used to assess rods against the fuel survival criteria, i.e. rods were sampled in the intervals shown in Table 4.8 and the effect of adjusting various geometry parameters were studied. The fuel survival criteria were:
• The maximum rod internal pressure must be below the coolant pressure, which was 15.5 MPa.

• The maximum clad hoop strain must be below 1%.

As was discussed in the previous chapter, the validity of ENIGMA’s results for average rod burnups above approximately 100 GW.d/tHM is questionable given that virtually no data exists to validate ENIGMA’s results for fuel rods above this burnup. This uncertainty is compounded by the fact that there is very limited data to validate (Th,U)O\(_2\) fuel rods. Hence, it was decided that only rods below 100 GW.d/tHM would be analysed with the assumption that if rods for a particular pin geometry fail at this threshold, then it is unlikely that rods at burnups above 100 GW.d/tHM would survive. Finally, none of the (Th,U,Gd)O\(_2\) rods were studied because relevant data on such fuel types appears, to date, to be non-existent and hence ENIGMA is currently incapable of modelling such fuel types.

ENIGMA currently only models axially-homogeneous (Th,U)O\(_2\) rods; however, as the majority of the rods (63%) have a single (Th,U)O\(_2\) content (due to the fact that the top and bottom regions are 1 cm and 90 cm respectively and the middle region constitutes the remaining 154.14 cm) it was decided to simply model the rod as if it was entirely made of the 154.14 cm material. A comparison was also made for rod C7-I306 using the axially-weighted-material contents within the rod, with the difference between the axially-weighted and non-axially weighted results being less than 1%. Hence, this assumption that the rods can be modelled by their largest single material constituent was considered appropriate.

The UO\(_2\) core designed in the previous chapter found that rods designed with an inner radius of up to 0.20 cm and a pellet-clad gap of 2.5g, where g = 8.2×10\(^{-3}\) cm (a standard pellet-clad gap size found in PWR fuel [16]) were sufficient to ensure the fuel survival criteria were obeyed. However, the data in Table 4.8 indicates that this rod geometry was insufficient and hence larger alterations in geometry were necessary. This implies that the (Th,U)O\(_2\) fuel inside the reactor designed in this study generally performed worse relative to UO\(_2\) fuel. In order to investigate whether this was the case it was decided to compare a sample of (Th,U)O\(_2\) rods from Table 4.8 with UO\(_2\) rods with identical power histories. Table 4.9 summarises the results from this comparison and shows considerably different behaviour between the sampled (Th,U)O\(_2\) rods and their equivalent UO\(_2\) rods. In order to assess why these differences in fuel behaviour have arisen it was decided to compare the various properties of one rod as a function of time.
<table>
<thead>
<tr>
<th>Pin ID</th>
<th>Burnup of solid pellet (GW.d/tHM)</th>
<th>Initial Gap Size (cm)</th>
<th>Inner radius of annulus (cm)</th>
<th>Plenum Length (cm)</th>
<th>Maximum Clad Hoop Creep Strain</th>
<th>Maximum Rod Internal Pressure (MPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C7-1306</td>
<td>99.998</td>
<td>2.5g</td>
<td>0.00</td>
<td>25.40</td>
<td>2.09%</td>
<td>13.17</td>
</tr>
<tr>
<td>C7-1306</td>
<td>99.998</td>
<td>3.5g</td>
<td>0.00</td>
<td>25.40</td>
<td>0.68%</td>
<td>15.89</td>
</tr>
<tr>
<td>C7-1306</td>
<td>99.998</td>
<td>3.5g</td>
<td>0.10</td>
<td>25.40</td>
<td>1.14%</td>
<td>14.09</td>
</tr>
<tr>
<td>C7-1306</td>
<td>99.998</td>
<td>4g</td>
<td>0.10</td>
<td>25.40</td>
<td>0.42%</td>
<td>15.27</td>
</tr>
<tr>
<td>C7-1306</td>
<td>99.998</td>
<td>3.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>3.02%</td>
<td>10.16</td>
</tr>
<tr>
<td>C7-1306</td>
<td>99.998</td>
<td>4g</td>
<td>0.20</td>
<td>25.40</td>
<td>1.41%</td>
<td>11.13</td>
</tr>
<tr>
<td>B6-0504</td>
<td>99.933</td>
<td>2.5g</td>
<td>0.00</td>
<td>25.40</td>
<td>1.74%</td>
<td>12.75</td>
</tr>
<tr>
<td>B6-0504</td>
<td>99.933</td>
<td>2.5g</td>
<td>0.10</td>
<td>25.40</td>
<td>2.35%</td>
<td>11.54</td>
</tr>
<tr>
<td>B6-0504</td>
<td>99.933</td>
<td>3.5g</td>
<td>0.10</td>
<td>25.40</td>
<td>0.28%</td>
<td>13.10</td>
</tr>
<tr>
<td>B6-0504</td>
<td>99.933</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>3.06%</td>
<td>10.50</td>
</tr>
<tr>
<td>B7-1217</td>
<td>99.559</td>
<td>2.5g</td>
<td>0.20</td>
<td>25.40</td>
<td>3.02%</td>
<td>9.98</td>
</tr>
<tr>
<td>B7-1217</td>
<td>99.559</td>
<td>4g</td>
<td>0.20</td>
<td>25.40</td>
<td>0.42%</td>
<td>11.37</td>
</tr>
<tr>
<td>B6-1310</td>
<td>84.747</td>
<td>2.5g</td>
<td>0.00</td>
<td>25.40</td>
<td>0.25%</td>
<td>8.61</td>
</tr>
<tr>
<td>C8-1606</td>
<td>84.453</td>
<td>2.5g</td>
<td>0.00</td>
<td>25.40</td>
<td>0.75%</td>
<td>8.18</td>
</tr>
<tr>
<td>A6-0406</td>
<td>84.234</td>
<td>2.5g</td>
<td>0.00</td>
<td>25.40</td>
<td>0.59%</td>
<td>8.64</td>
</tr>
<tr>
<td>A6-0406</td>
<td>84.234</td>
<td>2g</td>
<td>0.00</td>
<td>25.40</td>
<td>1.52%</td>
<td>8.32</td>
</tr>
<tr>
<td>B7-1601</td>
<td>59.941</td>
<td>1.5g</td>
<td>0.00</td>
<td>25.40</td>
<td>0.29%</td>
<td>5.65</td>
</tr>
<tr>
<td>B7-1601</td>
<td>59.941</td>
<td>1g</td>
<td>0.00</td>
<td>25.40</td>
<td>1.31%</td>
<td>5.39</td>
</tr>
<tr>
<td>A6-1104</td>
<td>59.520</td>
<td>1.5g</td>
<td>0.00</td>
<td>25.40</td>
<td>0.00%</td>
<td>5.67</td>
</tr>
<tr>
<td>A6-1210</td>
<td>59.124</td>
<td>1g</td>
<td>0.00</td>
<td>25.40</td>
<td>1.73%</td>
<td>5.32</td>
</tr>
</tbody>
</table>

Table 4.8: Sample of pins taken from different burnup bins (shaded rows). The Pin ID indicates the location of the fuel pin assessed within the core, with the first two characters referring to the assembly location and the remaining four digits indicating the pin location within an assembly from the bottom left hand corner in terms of row and column location, e.g. 0101 would indicate a fuel pin in the bottom left hand corner and 1717 a fuel pin in the top right hand corner. Burnups displayed are the average across the length of the rod and are from the SIMULATE run containing solid pellets, i.e. as pellet geometry is changed the effect on burnup has not been displayed in this table. The Initial Gap Size corresponds to the pellet-clad gap size at the beginning of life and is shown in terms of a multiple of g, where g = 8.2×10^−3 cm (1g is equal to the pellet-clad gap in a typical PWR rod [16]). The Plenum Length is the length of one of the rod’s plenums (there are plenums at the bottom and top of the rod of identical lengths), a larger plenum length will, for a given diameter, result in a larger volume to accommodate fission gases that have been released from the fuel matrix. The maximum clad hoop creep strain is the highest clad hoop creep strain across the entire rod, over the life of the rod. The rod internal pressure and clad hoop creep strain must be below 15.5 MPa and 1% respectively in order to ensure that the likelihood of rod failure is sufficiently low [20].
Table 4.9: Comparison of fuel performance characteristics for 6 rods sampled from Table 4.8 along with the behaviour of UO$_2$ rods run with identical power histories. The maximum clad hoop creep strain and the maximum rod internal pressure throughout life for (Th,U)O$_2$ rods are always greater than or equal to the same parameter for the UO$_2$ rods.

The chosen rod that was analysed in detail was rod C7-1306. Rod C7-1306 has a Th to (Th,U) content of 32.5%. ENIGMA reported that the maximum clad hoop creep strain occurred in axial zone 7 of 16. Therefore the following properties in axial zone 7 were analysed as a function of time: fuel radial temperature, fission gas release and clad hoop creep strain.

Figure 4.21: Radial temperature behaviour as a function of time for (Th,U)O$_2$ and UO$_2$ rods using the power history from rod C7-1306 in the optimised (Th,U)O$_2$ core. Temperature profiles are shown for axial zone 7 of 16 as this was found to be the location where maximum clad hoop creep strain occurred in the (Th,U)O$_2$ rod in Table 4.9. The sudden changes in fuel temperatures observed in both fuel types at around 7-8 years are due to changes in the power histories caused by relatively large movements in control rod positions; this would disappear if a finer step size was utilised and a narrower $k_{eff}$ convergence criterion was put in place.

Figure 4.21 shows how the temperature differs between the two rods as a function of time and pellet radial position. The outer radial position has been included as it is the thermal conductivity of the outer regions that matters most when deriving accurate temperature profiles of fuel rods, because thermal energy is transferred from the centre of the rod to the external coolant through these regions.
Therefore small differences in thermal conductivity of the outer regions between the two cases has a disproportionate impact on fuel temperature.

It was found that the temperature in the outer regions of both fuel types was roughly the same ($\sim 400^\circ$C). Figure 4.19, for a Th content of 32.5%, shows that ENIGMA will be predicting a slightly higher thermal conductivity for the UO$_2$ fuel relative to the (Th,U)O$_2$ fuel. This implies that the lower temperature observed in UO$_2$ is due to the fuel parameters (temperature and Th content) resulting in a UO$_2$ rod with improved thermal conductivity behaviour relative to (Th,U)O$_2$ fuel. In addition (as has been mentioned previously) the burnup in a (Th,U)O$_2$ fuel region will always be higher than an equivalent UO$_2$ fuel region outputting the same quantities of thermal energy, because the density of ThO$_2$ is significantly lower than UO$_2$ fuel. The higher burnup for the (Th,U)O$_2$ case will result in a degradation of thermal conductivity (discussed below).

Figure 4.21 also includes a magnified section of the outer fuel region temperature early on in rod life. This section of the plot shows that divergence in fuel temperatures starts to occur at around 3 years into rod life. The higher burnup of (Th,U)O$_2$ fuel relative to UO$_2$ fuel will result in greater swelling occurring in the (Th,U)O$_2$ fuel at a particular point in time, which will tend to increase the clad hoop creep strain.

The inventory of solid fission products is proportional to burnup and therefore their inventory in (Th,U)O$_2$ fuel will be higher than in the UO$_2$ at the same instance in time. As each uranium atom that fissions is in general replaced by two fission product atoms, the net effect is for swelling to increase as burnup increases. Hence, swelling will be higher in the (Th,U)O$_2$ region. As the pellet swells its temperature will increase. This is because higher fuel temperatures increase the amount of bubble formation and therefore result in an increase in porosity and therefore greater swelling. As porosity increases this will have a detrimental impact on thermal conductivity computed by ENIGMA, further increasing the fuel temperature and driving greater bubble formation (a positive feedback mechanism). Therefore, it is likely that the poorer thermal conductivity in the outer regions of the (Th,U)O$_2$ fuel and the degradation mechanisms related to burnup (namely degraded thermal conductivity and swelling) result in the large discrepancies between fuel temperatures.

Finally, there is also the effect of fuel creep to consider. ENIGMA currently assumes that the creep phenomena for (Th,U)O$_2$ fuel are identical to those for ThO$_2$ fuel, i.e. it does not factor in any dependence on U content. There appears limited data on the various creep rates for (Th,U)O$_2$ fuel. Hence, it is possible that ENIGMA is predicting unrealistic creep rates for the (Th,U)O$_2$ present in
the core studied here and hence the clad hoop creep strain predicted is too high. Nevertheless the lower \((\text{Th, U})\text{O}_2\) fuel creep relative to \(\text{UO}_2\) predicted by ENIGMA limits the ability of the \((\text{Th, U})\text{O}_2\) fuel to readily deform under high stress. This will result in the stress becoming concentrated in the clad, therefore further increasing clad hoop creep strain.

Figure 4.22: Clad hoop creep strain as a function of time for axial zone 7 of 16. The \((\text{Th, U})\text{O}_2\) and \(\text{UO}_2\) rod power histories were identical and taken from pin C7-1306 in Table 4.9. The larger clad hoop creep strain witnessed in the \((\text{Th, U})\text{O}_2\) fuel appears to be not only due to the greater amount of swelling occurring in the \((\text{Th, U})\text{O}_2\) fuel relative to the \(\text{UO}_2\) fuel but also the fact that fuel creep is much lower in \((\text{Th, U})\text{O}_2\) fuel. The lower fuel creep rates imply that once the pellet-clad gap has closed as stress is applied to the fuel from the high pressure coolant, the fuel is much less able to deform under the applied stress and therefore stress accumulates in the clad resulting in greater clad hoop creep.

Figure 4.22 shows the evolution of clad hoop creep in axial zone 7 for the \((\text{Th, U})\text{O}_2\) and \(\text{UO}_2\) fuel rods based on power histories taken from pin C7-1306. Pellet-clad gap closure occurs much earlier on in the \((\text{Th, U})\text{O}_2\) rod relative to the \(\text{UO}_2\) rod (6.8 years vs 9.3 years), which is due to the greater amount of swelling occurring in the \((\text{Th, U})\text{O}_2\) fuel. The earlier gap closure explains the sudden drop in \((\text{Th, U})\text{O}_2\) temperature shown in Figure 4.21. Once gap closure has occurred, clad hoop creep in the case of \((\text{Th, U})\text{O}_2\) rapidly increases in comparison to the \(\text{UO}_2\) rod clad hoop creep profile after closure has occurred. This supports the hypothesis that the low fuel creep rates for \((\text{Th, U})\text{O}_2\) are also a factor with respect to the higher observed clad hoop creep strain values.

Another surprising feature shown in Table 4.8 is that whilst employing annular pellets decreases rod internal pressure, the maximum clad hoop creep strains become larger relative to the solid pellet. This is different to the behaviour witnessed in the previous chapter when analysing \(\text{UO}_2\) rods, where annular pellets decreased both rod internal pressure and clad hoop creep strain. The reason for this
divergent behaviour appears to be because the creep phenomena occurring in the (Th,U)O\(_2\) pellets are lower than the UO\(_2\) pellet. In addition, the fact that lower fuel temperatures decrease creep rates will further decrease fuel creep in the annular (Th,U)O\(_2\) pellets. This will limit the ability of fuel to deform under the stress applied by the clad material.

In conclusion, it is the relatively low power density of the core, which is inherent in the long-life core design, that causes fuel temperatures to be lower than is normal and this happens to result in the thermal conductivity characteristics being better for the UO\(_2\) fuel than the (Th,U)O\(_2\) fuel. Furthermore, the relatively large difference in (Th,U)O\(_2\) fuel densities with significant amounts of Th present (>20%) implies that the burnup for an equivalent power history will be larger in (Th,U)O\(_2\) fuel compared to the UO\(_2\) fuel. Given the sensitivity of fuel degradation mechanisms to burnup this further explains why the (Th,U)O\(_2\) fuel generally shows poorer fuel performance characteristics relative to UO\(_2\). Data also currently suggests only the \(D_{th}\) component of the diffusion coefficient is lower in (Th,U)O\(_2\) fuel. This parameter only becomes important at very high fuel temperatures, in excess of 1400 K, which, given that the fuels tend to spend little time at such elevated temperatures during their lives, is of little benefit. In addition, the UO\(_2\) fuel appears to operate at significantly lower temperatures than the (Th,U)O\(_2\) fuel which will tend to result in lower fission gas release relative to the (Th,U)O\(_2\) fuel. Hence, for low power density cores operating at low temperatures the current data implies that the performance of thorium-based oxide fuels will be worse than UO\(_2\) fuels.

### 4.7 Economic Assessment

As two cores have been designed (a UO\(_2\) core and a (Th,U)O\(_2\) core) it was possible to perform an assessment of the fuel costs. Only uranium feedstock and enrichment costs were considered here as they tend to dominate fuel costs [179]. The thorium feedstock costs were initially ignored. Furthermore, given that the cores contain the same number of fuel rods the costs of reactor grade zirconium were ignored. It should be stated that in order to perform a fair cost comparison between the two cores more optimisation work would be required for both cores in order to achieve high confidence that the core loading pattern solutions for both core types are optimal.

The (Th,U)O\(_2\) core required 20.05 tonnes of uranium at an enrichment of 19.5 wt.%. At a cost of $66 per kg-U [179] and $90 per kg-Separative Work Unit [179], and assuming a tails concentration of 0.25 wt.%, this results in a total fuel cost of around $128 million. For comparison the UO\(_2\) core
had fuel costs of around $126 million. Hence, the (Th,U)O$_2$ core had comparable fuel costs to the UO$_2$ core. In addition, if the price of thorium were factored in at say the same price as the natural uranium, i.e. $66 per kg-Th, this would only add around $500 k to the price of the (Th,U)O$_2$ core.

4.8 Summary

Overall the neutronic characteristics of a thorium-fuelled core are very similar to the UO$_2$ core:

- Shutdown margins are in general comparable between the two cores.
- Xenon transients are significantly lower than the already small transients observed in the UO$_2$ core. However, this could be due to the harder spectrum due in part to the higher $^{235}$U content.
- Peak reactivity increase is significantly lower than in the UO$_2$ core ($\sim 370$ pcm vs $\sim 490$ pcm). However, this appears to be an artefact of the core returned by the discriminator algorithm rather than any inherent benefit caused by the presence of thorium in the fuel mixture.
- In general the Moderator Temperature Coefficients are slightly more negative throughout life although the Doppler coefficients are in general slightly more positive. Overall the difference for either sets of reactivity coefficients is not considered superior or inferior.

A comparison between MONK’s continuous nuclear data library and CASMO’s 70 group energy structure for a variety of comparable (Th,U)O$_2$ and UO$_2$ lattices showed that the discrepancy was significantly higher for the (Th,U)O$_2$ lattices. This implies that the multi-group structure employed in CASMO is not sufficient to accurately model (Th,U)O$_2$ lattices. However, it should be noted that for high gadolinium and/or high $^{235}$U enrichment lattices, both lattice types had discrepancies greater than 1% between MONK and CASMO.

Fuel performance is in general worse relative to equivalent UO$_2$ rods for the reactor being studied in this investigation. This is likely due to the fact that for low fuel temperatures ($\lesssim 600^\circ$C), with uranium content in the range 35 to 75 wt.%, the thermal conductivity is lower in (Th,U)O$_2$ fuel than UO$_2$ fuel. In addition, the burnup will always be higher in (Th,U)O$_2$ fuel than UO$_2$ for a given power history due to the lower density of ThO$_2$ fuel. This results in higher swelling and greater thermal conductivity degradation in the case of (Th,U)O$_2$ fuel relative to UO$_2$ fuel. Hence, overall fission gas release and rod internal pressure were higher in the case of (Th,U)O$_2$ fuel relative to UO$_2$. 

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fuel. Furthermore, creep is in general lower for thorium-based fuels which is unfavourable as creep is important in reducing stress concentration between the clad and the fuel pellet. Hence, ENIGMA predicted that the clad hoop creep strain is significantly higher in the case for the (Th,U)O$_2$ rods. However, there are considerable uncertainties regarding a variety of fuel parameters that are required to accurately model (Th,U)O$_2$, these include:

- Limited burnup performance data, in particular thermal conductivity degradation as a function of burnup.
- Data on $D_{\text{mix}}$ and $D_{\text{ath}}$ diffusion coefficients appears non-existent.
- Data on creep rates as a function of uranium content in (Th,U)O$_2$ fuel appears very limited.

In addition, whilst there is quite considerable information on (U,Gd)O$_2$ fuel parameters up to approximately 15 wt.% Gd, the data on (Th,U,Gd)O$_2$ appears to be very limited. Therefore whilst the (Th,U)O$_2$ core contained significantly lower gadolinia content it is not possible to assess the fuel performance benefits for such fuels. The above highlights deficiencies in the current (Th,U)O$_2$ datasets that should be addressed in order to permit accurate comparisons between (Th,U)O$_2$ and UO$_2$ fuel.

An economic assessment between the fuel costs of the UO$_2$ core vs the (Th,U)O$_2$ core found the (Th,U)O$_2$ core to have a comparable costs to the UO$_2$ core fuel costs. However, it should be stated that in order to perform a fair cost comparison between the two cores more optimisation work would be required for both cores in order to achieve high confidence that the core loading pattern solutions for both core types are optimal.
Chapter 5

Validation of MONK for Thermal $^{233}\text{U}/^{232}\text{Th}$ Systems

5.1 Outline

Nuclear data is available in a number of forms, which are typically [89]:

- Cross-section data from a variety of experiments, which may have different degrees of accuracy and give different values for the same cross-sections.
- Different theoretical calculations of varying accuracy.

The above data types form the basis of so-called evaluated nuclear data files. In order to achieve this the various data types must be checked for consistency and normally any gaps in the data are filled using existing theories or educated guesses [89].

<table>
<thead>
<tr>
<th>Nuclear Data Library</th>
<th>Year Released</th>
<th>Available in MONK version</th>
</tr>
</thead>
<tbody>
<tr>
<td>JEF 2.2</td>
<td>1992</td>
<td>MONK-9A and MONK-10A</td>
</tr>
<tr>
<td>JEFF 3.1</td>
<td>2005</td>
<td>MONK-10A</td>
</tr>
<tr>
<td>JEFF 3.1.1</td>
<td>2009</td>
<td>MONK-10A</td>
</tr>
<tr>
<td>JEFF 3.1.2</td>
<td>2012</td>
<td>MONK-10A</td>
</tr>
</tbody>
</table>

Table 5.1: JEF/P libraries available in the current MONK version (MONK-9A) and the next MONK release (MONK-10A) [21].
In all of the previous chapters the models constructed have used the JEF (Joint Evaluated File) 2.2 nuclear data library. This has been used heavily to date in designing and licensing reactors in Europe although there are a variety of libraries including ENDF/B used predominantly in the United States and CENDL used in China [89]. The JEF 2.2 nuclear data library was initially released in 1992, subsequent revisions to this nuclear data library have been made resulting in the next version of MONK-10A incorporating more recent JEFF (Joint Evaluated Fission and Fusion file) 3.1, 3.1.1 and 3.1.2 nuclear data libraries (see Table 5.1).

To date there has been little validation for MONK performed on $^{232}$Th/$^{233}$U systems and whilst a series of $^{232}$Th/$^{233}$U experiments have been modelled in MCNP these have tended to employ older nuclear data libraries (versions of ENDF/B-V and earlier which were released prior to 1979 [15]) [180]. The comparisons that have been performed have often been done in isolation - i.e. very limited analysis has been carried out assessing the performance of a particular code using a consistent library to model a series of different $^{232}$Th/$^{233}$U experiments. Furthermore, limited analysis has been performed with more recent nuclear libraries, in particular with versions of JEF 2.2 and later versions. This chapter therefore examines the discrepancy between MONK-9A simulations and a series of different experiments that have incorporated $^{232}$Th and/or $^{233}$U, both with JEF 2.2 and with a newer developmental JEF/F release available at the time of undertaking this validation which was the JEFF 3.1 nuclear data library. The main difference between the developmental version of JEFF 3.1 used in this study and the final release version was that the nuclear data in the developmental version is only available for materials at 293 K (room temperature). This temperature limitation turned out to be sufficient for the experiments investigated here as all were performed at room temperature, i.e. $\sim 293$ K.

The experiments modelled were taken from a series of reports from the International Criticality Safety Benchmark Evaluation Project (ICSBEP) [180]. The primary purpose of the ICSBEP is to “compile benchmark experiment data into a standardised format that allows analysts to easily use the data to validate calculational techniques and cross-section data” [181].

The ICSBEP evaluators assess the experimental data to determine whether sufficient information is available to construct a viable benchmark, for example they ensure that all of the necessary information with respect to geometry and constituent materials has been reported with sufficient accuracy. From there a so-called benchmark model is created. These benchmark models simplify the experimental descriptions by neglecting most components that do not significantly affect the $k_{\text{eff}}$ of the system.
such by homogenising individual components of a core’s structure, for example mechanical joints with
the surrounding material. The effects of these simplifications on the experimental $k_{\text{eff}}$ ($k_{\text{exp}}$) are
determined and result in a bias. Hence the benchmark $k_{\text{eff}}$ ($k_B$) is defined as

$$k_B = k_{\text{exp}} + \text{bias} \pm \sqrt{u_{\text{exp}}^2 + u_{\text{bias}}^2}$$  \hspace{1cm} (5.1)

where $u_{\text{exp}}$ and $u_{\text{bias}}$ are the uncertainties attached to the experimental measurement and the intro-
duced bias respectively.

The key parameter of interest when assessing the performance of a particular code using a specific
nuclear data library is the discrepancy between the calculated $k_{\text{eff}}$ ($k_C$) from the utilised code and $k_B$.
Hence the discrepancy is defined as

$$\frac{k_C - k_B}{k_B}$$  \hspace{1cm} (5.2)

where the uncertainty from the discrepancy is the combined uncertainty from the statistical Monte
Carlo uncertainty from $k_C$ and the uncertainty from $k_B$ shown in Equation 5.1.

In some of the ICSBEP reports detailed here there were two types of benchmark models, termed
simplified and detailed, with the former containing larger degrees of model simplification. This present
examination lists the results from the detailed cases only. The chosen experiments to model were
selected on the basis that the uncertainty in $k_B$ was less than or equal to ±0.005. This level of
uncertainty was low enough to permit a variety of systems to be studied but was deemed not so high
that discrepancies could be hidden by the associated uncertainty.

Four sets of benchmark experiments were implemented in the current version of MONK (MONK-
9A). These were:

1. A series of uranyl nitrate $\text{UO}_2(\text{NO}_3)$ solution experiments contained within spherical vessels,
with the predominant fissile material being $^{233}\text{U}$. These experiments were performed by Oak
Ridge National Laboratory over the period 1950 to 1968 [35, 36, 182]. The purpose of these
experiments was to provide information applicable to criticality safety practices, analyse basic
geometry configurations and determine $\eta_{\text{th}}$ (the average number of neutrons released per thermal
neutron absorbed).

2. The Thorium Uranium Physics Experiments (TUPE) which consisted of studying a series of
cores with each core containing thorium and highly enriched uranium-235 oxide fuel rods. The fuel rods were surrounded by light water coolant with various concentrations of boron [22]. These experiments were performed at the Babcock & Wilcox facilities in Lynchburg, Virginia from 1959-1960 for the Atomic Energy Commission [22]. The purpose of these experiments was to determine various physics parameters including critical sizes and masses, non-leakage probabilities and the contribution of thermal and fast neutrons to $k_{\infty}$ [22].

3. RBMK core experiments that consisted of Low Enriched Uranium (LEU) oxide and metallic thorium pellets residing within the graphite-moderated systems that had fuel channels either flooded or unflooded with light water. These experiments were performed over the period 1982-1988 at the Kurchatov Institute relating to RBMK research and development [37].

4. A series of critical experiments that were to support the development of the breeder blankets for the Light Water Breeder Reactor (LWBR). These experiments consisted of uranium-zirconium oxide and thorium-uranium oxide fuel rods surrounded by light water with the predominant fissile nuclides being $^{233}$U and $^{235}$U [183]. The experiments were performed in the mid-1960s at the High Temperature Test Facility of the Bettis Atomic Power Laboratory (BAPL) in West Mifflin, Pennsylvania by Westinghouse Atomic Power Division [183].

The referenced reports provide all of the analysis and detail regarding the construction of the associated benchmark models, in particular the determined biases and uncertainties. Hence to aid traceability the original names for the benchmark models from these reports are also included in the work detailed here. To avoid unnecessary duplication of the referenced reports only the main differences between the original experiments and the benchmark are highlighted.

All benchmark models were performed at 293 K and while some experiments did have slightly elevated temperatures (up to around 303 K), the main effect of this, from a reactivity perspective, would have been to alter the density of the moderators. The benchmark models incorporate density changes as a function of temperature and therefore any remaining differences such as underestimation in Doppler broadening we have deemed negligible.

All results were analysed in terms of the magnitude of the discrepancy, in particular whether or not the discrepancy is $< 0.5\%$ and $> 1.0\%$, and any statistically significant difference between the experimental and calculated $k_{\text{eff}}$s. Discrepancies of $< 0.5\%$ and $> 1.0\%$ are respectively viewed in licensing activities as showing good and poor agreement with experimental and calculated $k_{\text{eff}}$s [184].
In the study any difference between the experimental and calculated values of greater than 2 $\sigma$ (where $1 \sigma$ equals 1 standard deviation) is viewed as being statistically significant.

All of the systems modelled contain moderators (primarily light water ($\text{H}_2\text{O}$)) and therefore a way to distinguish between the different models is necessary. Furthermore, the primary constituents of these systems contain Hydrogen (H) and Heavy Metals (HM), where the term heavy metals refers to elements with atomic numbers greater than actinium. A key difference between hydrogen and heavy metals is the number of elastic collisions required to reduce a neutron energy from birth (around 2 MeV) to thermal energies (around 1 eV). In the case of hydrogen nuclei only around 14 collisions on average are required to reduce a neutron’s energy from 2 MeV to 1 eV, whereas in the case of $^{238}\text{U}$ around 1700 elastic collisions are required [89]. Therefore the parameter H:HM can be used to determine the degree of thermalisation within systems where the moderator is light water. Furthermore, only the amounts of hydrogen and heavy metal present within the active-moderated region has been used in determining the H:HM values for the systems investigated in this study, with hydrogen present in the reflector ignored in calculating H:HM. The reason for ignoring hydrogen present in the reflector is that neutrons travel a relatively short distance in water [183] and therefore it is nonsensical to simply include the total amount of hydrogen within the reflector in the H:HM value. If the hydrogen content within the reflector were to be included when determining H:HM, it would be necessary to calculate the relative importance of the reflector in each system; for example, a system with a large proportion of neutrons entering the reflector would have a neutron flux that is more sensitive to the hydrogen content within the reflector than a system with a limited number of neutrons entering the reflector. Hence ideally a system dependent weighting factor would be applied to the proportion of hydrogen within the reflector dependent upon the neutron leakage rate. By ignoring the hydrogen content of the reflector in the H:HM calculation we avoid these complications. However, for completeness the geometry and/or volume of water reflectors is specified in the description associated with each of the systems modelled.

Note that in the case of the RBMK systems the volume of water within the systems is varied and the primary moderator is graphite (carbon). Neither H:HM nor C:HM are sufficient to quantify the degree of thermalisation\(^1\). Therefore within this analysis this parameter is not utilised and instead RBMK systems are differentiated from one another by the presence of light water within the active

\(^1\)It is tempting to use a hybrid parameter such as $(\text{H}+\text{C})$:HM; however, this brings into question the weighting that should be applied to H and C as characteristics of these two moderators are different from one another.
region of the core.

The data from each series of the four series of experiments are initially analysed in terms of the dependence of the discrepancy on the degree of thermalisation. Then the overall discrepancy dependence is discussed once all calculations have been performed on the four sets of experiments.

### 5.2 Spherical Vessels Containing Uranyl Nitrate ($^{233}$UO$_2$(NO$_3$)$_2$)

Three sets of spherical vessel experiments were modelled containing a uranyl nitrate ($^{233}$UO$_2$(NO$_3$)$_2$) solution, taken from Refs.[35, 36, 182]. $^{233}$U accounted for more than 97 wt.% of the uranium in the solutions and all vessels were constructed of aluminium type 1100. The three experiments were:

1. Unreflected spheres of $^{233}$U nitrate solution [35];
2. Light water reflected spherical vessels partially filled and filled with $^{233}$U nitrate solution [36];
3. Unreflected spherical vessels partially filled and filled with $^{233}$U nitrate solution [182].
Figure 5.1: The experimental setup for the experiment consisting of unreflected spheres of $^{233}\text{U}$ nitrate solution. Taken from [35].

Figure 5.1 shows an example of one of the experimental arrangements. All of the experiments utilised a similar experimental setup with the main differences being the constituents of the uranyl nitrate solution, the size of the spherical vessel (along with the volume of uranyl nitrate solution within the vessel) and whether or not the spherical vessels were surrounded by light water.
Figure 5.2: Benchmark model for the reflected system with dimensions in cm. A was varied between 17.9645 cm and 28.740 cm, B was varied between 11.1768 cm and 14.6232 cm and 65.8 cm and 68.5 cm (note that the number of significant figures does not represent the accuracy and is only included to convert back to the original dimensions which were in inches). Taken from [36].

Figure 5.2 shows the benchmark model for the reflected system, which was considerably more detailed than the unreflected systems as it included the tank the vessel was within, support plates and pipe work. Hence no bias was introduced in the reflected system benchmark model. However, the unreflected systems only included the spherical vessels the solutions resided within, and therefore a bias of up to -0.0008 was introduced. This bias was due to ignoring the surrounding structural materials which had the effect of reflecting a small proportion of neutrons back into the system (referred to as room return) [35, 182].

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Table 5.2 gives the details on the cases modelled from Refs. [35, 36, 182]. Cases were selected on the basis of $k_B$ having an uncertainty of less than or equal to $\pm 0.005$ and also giving a variety of $H:HM$ ratios.

<table>
<thead>
<tr>
<th>ID</th>
<th>Reference in Reference</th>
<th>Case Name</th>
<th>Volume (l)</th>
<th>H:HM</th>
<th>Reflected</th>
<th>Boric Acid Concentration (mg/g)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>[36]</td>
<td>1</td>
<td>5.33</td>
<td>$1.18 \times 10^2$</td>
<td>Yes</td>
<td>0.00</td>
</tr>
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<td>[36]</td>
<td>2</td>
<td>5.48</td>
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<td>0.00</td>
</tr>
<tr>
<td>3</td>
<td>[36]</td>
<td>3</td>
<td>5.67</td>
<td>$1.37 \times 10^2$</td>
<td>Yes</td>
<td>0.00</td>
</tr>
<tr>
<td>4</td>
<td>[36]</td>
<td>4</td>
<td>5.90</td>
<td>$1.86 \times 10^2$</td>
<td>Yes</td>
<td>0.00</td>
</tr>
<tr>
<td>5</td>
<td>[36]</td>
<td>6</td>
<td>7.11</td>
<td>$2.64 \times 10^2$</td>
<td>Yes</td>
<td>0.00</td>
</tr>
<tr>
<td>6</td>
<td>[36]</td>
<td>7</td>
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<td>[182]</td>
<td>9</td>
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</tr>
<tr>
<td>9</td>
<td>[182]</td>
<td>10</td>
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<td>$1.81 \times 10^2$</td>
<td>No</td>
<td>0.00</td>
</tr>
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<td>10</td>
<td>[182]</td>
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<td>$1.30 \times 10^1$</td>
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<td>11</td>
<td>[182]</td>
<td>18</td>
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<td>0.00</td>
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<td>[182]</td>
<td>21</td>
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<td>[35]</td>
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</tr>
<tr>
<td>14</td>
<td>[35]</td>
<td>2</td>
<td>$1.73 \times 10^2$</td>
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<td>0.0233</td>
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<td>3</td>
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<td>[35]</td>
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</tr>
<tr>
<td>17</td>
<td>[35]</td>
<td>5</td>
<td>$1.73 \times 10^2$</td>
<td>$1.29 \times 10^3$</td>
<td>No</td>
<td>0.0887</td>
</tr>
</tbody>
</table>

Table 5.2: Details of the main differences between the 17 uranyl nitrate solution experiments modelled in this study.

These 17 models were run using the BINGO - JEF 2.2 and BINGO - JEFF 3.1 libraries. Figures 5.3 and 5.4 show the discrepancies vs $H:HM$ ratios.
It can be seen in Figure 5.3 that there is some dependence of discrepancy on H:HM ratio for the less thermalised systems. This is especially true when it is factored in that the reflected systems will be more thermalised than their H:HM ratio from the solutions implies, as some neutrons will be interacting with hydrogen in the surrounding water reflector and returning to the system, thereby further softening the spectrum. However, Figure 5.4 appears to show no obvious correlation between discrepancy and H:HM ratio. In fact all calculated $k_{\text{eff}}$s are within 2 standard deviations of each other, whereas for the BINGO - JEF 2.2 runs this is only true for the heavily thermalised systems from Ref. [35].

In conclusion, the majority of the JEFF 3.1 runs have discrepancies less than 0.5%; however, for the JEF 2.2 runs this is only true for the highly thermalised systems (H:HM > 1200).
5.2.1 Thorium Uranium Physics Experiments

The experiments modelled here consisted of cores containing an array of fuel pins with an active length in all cases of 152.40 cm (60 in.). The rods were placed within the core in a circular arrangement. Figure 5.5 gives an example of one of the core layouts. From the original series of experiments Ref. [22] deemed 100 experimental configurations to contain sufficient information to create benchmark cases. Of the 100 configurations approximately two thirds of them contained borated water.

The original experiments differed from one another by the following parameters:

- Concentration of boron present in light water coolant/reflector;
- Radial dimensions of the fuel rods (of which there were two types - see Figure 5.7);
- Critical height of water within the tank the experiment was carried out in;
- Number of fuel rods present within the tank;
- The relative mixture of uranium oxide and thorium oxide within the fuel rods (of which there were two types - see Table 5.3).

![Figure 5.5: Example of one of the uniform thorium-uranium oxide lattice layouts modelled in this investigation. Taken from [22].](image)

Figure 5.6 displays the vertical view of a benchmark model based on this series of experiments.
Figure 5.6: Vertical view of the benchmark model for the thorium-uranium lattice cores modelled in this investigation, with dimensions in cm. Taken from [22].

(a) Radial slice of type 1 fuel rod.

(b) Radial slice of type 2 fuel rod.

Figure 5.7: Dimensions for the two distinct rod types containing material mixtures shown in Table 5.3, taken from [22]. There were two different pellet sizes used in this experiment with diameters of 0.5944 cm (0.234 in.) and 0.6604 cm (0.260 in.). The fuel rod diameter was the same in all cases, which was 0.7849 cm (0.309 in.), but the Al clad and gap thickness were varied to accommodate the different pellet sizes.

The experiments consisted of two distinct fuel rod types (referred to here as Type 1 and Type 2 rods). The geometry of Types 1 and 2 are shown in Figures 5.7a and 5.7b respectively. Not only did the dimensions of these two rod types differ but their contents were also different. Table 5.3 shows the key composition differences between the two rod types.
Table 5.3: Information on the contents of the two fuel matrix types from the uniform thorium-uranium oxide experiments. Both fuel types contained a uranium oxide mixture consisting of 62% of the U in the form of $\text{UO}_2$ and 38% is in the form of $\text{U}_3\text{O}_8$.

<table>
<thead>
<tr>
<th>Fuel Property</th>
<th>Type 1</th>
<th>Type 2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{238}\text{U}$ in uranium oxide mixture</td>
<td>0.33 wt.%</td>
<td>0.26 wt.%</td>
</tr>
<tr>
<td>$^{235}\text{U}$ in uranium oxide mixture</td>
<td>5.59 wt.%</td>
<td>3.45 wt.%</td>
</tr>
<tr>
<td>$^{232}\text{Th}$ in $\text{ThO}_2$</td>
<td>83.89 wt.%</td>
<td>87.42 wt.%</td>
</tr>
<tr>
<td>Fuel Density (g/cm$^3$)</td>
<td>8.33</td>
<td>8.44</td>
</tr>
</tbody>
</table>

Table 5.4: Details of the 20 uniform thorium-uranium oxide experiments modelled along with the original case names in Ref. [22].

<table>
<thead>
<tr>
<th>ID</th>
<th>Case Name</th>
<th>No. of Pins</th>
<th>H:HM</th>
<th>Boron concentration (g/l)</th>
<th>Water Height (cm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>6</td>
<td>1968</td>
<td>4.85</td>
<td>0</td>
<td>44.08</td>
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<td>2</td>
<td>13</td>
<td>1108</td>
<td>4.85</td>
<td>0</td>
<td>116.19</td>
</tr>
<tr>
<td>3</td>
<td>14</td>
<td>1576</td>
<td>5.78</td>
<td>0.07</td>
<td>46.34</td>
</tr>
<tr>
<td>4</td>
<td>22</td>
<td>968</td>
<td>5.78</td>
<td>0.07</td>
<td>127.63</td>
</tr>
<tr>
<td>5</td>
<td>23</td>
<td>2000</td>
<td>5.78</td>
<td>0.322</td>
<td>43.8</td>
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<tr>
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<td>31</td>
<td>1160</td>
<td>5.78</td>
<td>0.322</td>
<td>129.29</td>
</tr>
<tr>
<td>7</td>
<td>32</td>
<td>2496</td>
<td>5.78</td>
<td>0.586</td>
<td>42.64</td>
</tr>
<tr>
<td>8</td>
<td>43</td>
<td>1364</td>
<td>5.78</td>
<td>0.586</td>
<td>124.6</td>
</tr>
<tr>
<td>9</td>
<td>44</td>
<td>2884</td>
<td>5.78</td>
<td>0.823</td>
<td>43.87</td>
</tr>
<tr>
<td>10</td>
<td>53</td>
<td>1552</td>
<td>5.78</td>
<td>0.823</td>
<td>127.07</td>
</tr>
<tr>
<td>11</td>
<td>54</td>
<td>820</td>
<td>10.4</td>
<td>0</td>
<td>43.56</td>
</tr>
<tr>
<td>12</td>
<td>62</td>
<td>540</td>
<td>10.4</td>
<td>0</td>
<td>102.41</td>
</tr>
<tr>
<td>13</td>
<td>63</td>
<td>540</td>
<td>10.4</td>
<td>0.235</td>
<td>42.69</td>
</tr>
<tr>
<td>14</td>
<td>71</td>
<td>672</td>
<td>10.4</td>
<td>0.235</td>
<td>104.6</td>
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<td>72</td>
<td>1632</td>
<td>10.4</td>
<td>0.432</td>
<td>38.25</td>
</tr>
<tr>
<td>16</td>
<td>81</td>
<td>840</td>
<td>10.4</td>
<td>0.432</td>
<td>109.4</td>
</tr>
<tr>
<td>17</td>
<td>82</td>
<td>2196</td>
<td>10.4</td>
<td>0.635</td>
<td>35.72</td>
</tr>
<tr>
<td>18</td>
<td>93</td>
<td>976</td>
<td>10.4</td>
<td>0.635</td>
<td>134.58</td>
</tr>
<tr>
<td>19</td>
<td>94</td>
<td>1500</td>
<td>12.6</td>
<td>0</td>
<td>69.85</td>
</tr>
<tr>
<td>20</td>
<td>100</td>
<td>1192</td>
<td>12.6</td>
<td>0</td>
<td>132.83</td>
</tr>
</tbody>
</table>

Table 5.4: Details of the 20 uniform thorium-uranium oxide experiments modelled along with the original case names in Ref. [22].

Of these 100 configurations, 20 were selected for modelling in MONK-9A. These 20 configurations were selected on the basis of having an uncertainty in $k_B$ of less than or equal to 0.005 and giving a variety of cores with different pellet sizes, compositions and core sizes. The number of rods present in the 20 experimental configurations investigated here varied between 540 to 2884, with the water height altered between cases from 35.72 to 134.58 cm relative to the bottom of the active length of the rods. All benchmark models included a 100 cm radial reflector around the core$^2$. Table 5.4 gives

$^2$In reality a light water reflector greater than approximately 30 cm can be viewed as infinitely large from the neutrons' perspective since the probability of a neutron travelling such a distance without being absorbed is effectively zero [183].
detailed information on each of the 20 configurations modelled in this investigation.

Figure 5.8: Discrepancy as a function of H:HM content for uniform thorium-uranium oxide lattices segregated by moderator/reflector type (borated or unborated) using the JEF 2.2 nuclear data library.

Figure 5.9: Discrepancy as a function of H:HM content for uniform thorium-uranium oxide lattices segregated by moderator/reflector type (borated or unborated) using the JEFF 3.1 nuclear data library.

The main difference between the actual experiments and the benchmark models were that some impurities within the two fuel types were ignored such as C, Si, Ca, Mn and Fe [22]. However, impurities with a large thermal absorption cross-section and relatively large abundances within the fuel (i.e. B and Gd) were included in the benchmark models. This resulted in a bias of around 0.0008. Also, the benchmark models did not include materials that surrounded the tank. This was because the tank was sufficiently large that room return was considered negligible.
Figures 5.8 and 5.9 shows the discrepancies as a function of H:HM content using the JEF 2.2 and JEFF 3.1 nuclear data libraries respectively. The lattices were divided into borated and unborated depending on the moderator/reflector conditions employed in the experiments. This was because it was expected that the borated lattices would exhibit a harder spectrum relative to the unborated cases with a similar H:HM ratio, as boron is a strong absorber of thermal neutrons.

Figures 5.8 and 5.9 suggest the discrepancies are broadly similar when using JEF 2.2 and JEFF 3.1 data libraries, i.e. there does not appear to be any significant reduction in the size of the discrepancies when utilising either nuclear data library. In fact the number of statistically significant results is the same for both data libraries (8 out of the 20 cases have discrepancies > 2σ, with 6 and 2 coming from borated and unborated lattices respectively).

5.3 RBMK System Containing Thorium Channels

RBMK reactors are a type of light-water-cooled graphite-moderated reactor that use water as a coolant and graphite, in addition to water, for moderation [167]. They have an operating capacity of 1 GWe.

A number of neutron experiments were performed at the Kurchatov Institute relating to RBMK research and development. Different critical masses were investigated in the RBMK Critical Facility. All experiments were performed at room temperature, with the maximum power of the RBMK Critical Facility being 25 watts. In addition, all elements within the facility’s core were identical to the elements in commercial RBMK reactors, except that the height of the core is half that of the 1 GWe power version [37].

The survey that this validation exercise is based on originally consisted of 28 critical experiments. These 28 experiments had different geometrical configurations of LEU, flooded and unflooded fuel channels, boron absorbers and thorium fuel [37]. We have focused just on the LEU and thorium fuel configurations, which constituted 12 critical experiments.

Figure 5.11a shows the layout of one of the 12 cores modelled in this study and Figure 5.11b shows a 3D output for the same core from MONK. Appendix D.1 shows the layout of all of the configurations modelled in this study. Each of the 12 models differ in the number of fuel channels, whether the fuel channels were flooded, and the layout of the fuel channels.

The benchmark model consisted of an 18 by 18 array of vertical aluminium channels, each surrounded by graphite. The channels were on a 25 cm square pitch. Within the centre of the core were
channels containing uranium oxide fuel enriched to 2 wt.% $^{235}$U. In some cases these channels were either all flooded or unflooded. Some of the cases that were modelled also contained metallic thorium pellets individually clad in aluminium. The entire core had dimensions of 450 cm by 450 cm in width and length, and 410 cm in height.

(a) 2D cross-section of Core 10. Note that the core graphite had around 1% fewer Cd and B impurities.

(b) 3D diagram of Core 10.

Figure 5.11: 2D and 3D diagrams of Core 10 which contains LEU (2 wt.% $^{235}$U) fuelled channels and thorium channels.

The UO$_2$ pellets and thorium metallic pellets had diameters of 2.296 cm and 3.49 cm respectively. The UO$_2$ pellets were stacked to a height of 345.14 cm, with each assembly containing 18 fuel pins (see Figure 5.10a). The fuel pins were arranged as two concentric rings, with the inner ring containing 6 fuel pins and the outer ring containing the remaining 12 pins. The metallic thorium pellets were stacked to a height of 348.5 cm (see Figure 5.10b).
(a) Vertical view of the benchmark model UO$_2$ fuel assembly.

(b) Vertical view of the benchmark model thorium fuel channel.

Figure 5.10: Vertical views of the benchmark model UO$_2$ fuel assemblies and thorium fuel channels. Taken from [37].
The main difference between the actual experiments and the benchmark models were that the benchmark models ignored the surrounding structural material, in particular the concrete beneath the support plate and borated plastic shielding material. The net effect of ignoring these external materials was a bias of up to -0.0008 [37].

Figure 5.12: Discrepancy for LEU cores which contain no thorium channels. Odd and even core IDs correspond to flooded and unflooded fuel channels respectively.

Figure 5.12 and Figure 5.13 show the discrepancies for the cores containing no thorium channels, and cores containing thorium channels, respectively. All of the odd core IDs contained flooded LEU fuel channels and all of the even core IDs were unflooded.

None of the JEFF 3.1 results had discrepancies > 1% and all but one of the JEFF 3.1 flooded cases had discrepancies less than 0.5%, whereas only the flooded JEF 2.2 cases had no discrepancies greater than 1%. Furthermore, all of the unflooded fuel channels for both JEF/F libraries gave statistically significant results. In addition, discrepancies were very similar with and without thorium. Therefore, the presence of thorium is unlikely to be a factor in the relatively large discrepancies for the unflooded fuel channel cases.
5.4 Zero Power Experiments from the Light Water Breeder Reactor Programme

In Ref. [183] eight cores are detailed and analysed from a set of critical experiments undertaken as part of the Light Water Breeder Reactor (LWBR) Programme conducted in the mid-1960s, with all eight cores modelled here. Table 5.5 gives details of the eight cores along with core IDs which are identical to those in Ref. [183]. With the exception of one core all cores had a central ‘seed’ region consisting of fuel rods containing high concentrations of fissile material, either $^{233}$U or $^{235}$U, that were surrounded by a blanket made up of fuels rods containing large amounts of thorium. The exception (core SB-2.5) contained only a seed region, i.e. no blanket was present. The cores had either rectangular or hexagonal geometries, with the seven cores containing a blanket having widths and lengths of approximately 60 cm×60 cm. The rod pitches were 0.91948 cm (0.362 in.) and 1.83896 cm (0.724 in.) in the seed and blanket regions for the rectangular geometry cores, with the hexagonal geometry cores having both a seed and blanket pitch of 1.45034 cm (0.571 in.). Figure 5.14 details one of the core configurations, along with key dimensions.

All fuel rods had an active length of 38.1 cm (15 in.). There were four fuel mixtures used within this set of experiments, which are detailed in Table 5.6 along with the rod cross-sectional dimensions. Two of these mixtures were used in the seed rods and consisted of either $^{233}$UO$_2$-ZrO$_2$ or $^{235}$UO$_2$-ZrO$_2$. The blanket rods contained either ThO$_2$ or $^{233}$UO$_2$-ThO$_2$. All fuel rods were clad in Zircaloy-2.
<table>
<thead>
<tr>
<th>Core ID</th>
<th>Core geometry</th>
<th>Seed rod material</th>
<th>Blanket rod material</th>
</tr>
</thead>
<tbody>
<tr>
<td>SB-1</td>
<td>Rectangular</td>
<td>$^{235}\text{UO}_2$-$\text{ZrO}_2$</td>
<td>ThO$_2$</td>
</tr>
<tr>
<td>SB-2</td>
<td>Rectangular</td>
<td>$^{235}\text{UO}_2$-$\text{ZrO}_2$</td>
<td>ThO$_2$</td>
</tr>
<tr>
<td>SB-2.5</td>
<td>Rectangular</td>
<td>$^{235}\text{UO}_2$-$\text{ZrO}_2$</td>
<td>NA</td>
</tr>
<tr>
<td>SB-3</td>
<td>Rectangular</td>
<td>$^{233}\text{UO}_2$-$\text{ZrO}_2$</td>
<td>$^{233}\text{UO}_2$-$\text{ThO}_2$</td>
</tr>
<tr>
<td>SB-4</td>
<td>Rectangular</td>
<td>$^{235}\text{UO}_2$-$\text{ZrO}_2$</td>
<td>$^{233}\text{UO}_2$-$\text{ThO}_2$</td>
</tr>
<tr>
<td>SB-5</td>
<td>Hexagonal</td>
<td>$^{235}\text{UO}_2$-$\text{ZrO}_2$</td>
<td>ThO$_2$</td>
</tr>
<tr>
<td>SB-6</td>
<td>Hexagonal</td>
<td>$^{235}\text{UO}_2$-$\text{ZrO}_2$</td>
<td>ThO$_2$</td>
</tr>
<tr>
<td>SB-7</td>
<td>Hexagonal</td>
<td>$^{233}\text{UO}_2$-$\text{ZrO}_2$</td>
<td>$^{233}\text{UO}_2$-$\text{ThO}_2$</td>
</tr>
</tbody>
</table>

Table 5.5: Information on the constituents and geometries of the eight seed and blanket cores.

Figure 5.14: LWBR benchmark seed-and-blanket core diagram. The yellow rods correspond to fertile bearing fuel rods in the blanket region of the core and the red rods correspond to fissile bearing fuel rods in the seed region of the core.

The cores also contained four control blades made of borated steel, with each blade having a thickness of 0.1778 cm (0.070 in.) and a width of 7.62 cm (3 in.), placed within the seed region. The control blades only penetrated approximately 8% into the active fuel region.

<table>
<thead>
<tr>
<th>Matrix</th>
<th>U wt.% in material</th>
<th>$^{235}\text{U}$ or $^{239}\text{U}$ wt.% in material</th>
<th>Fuel rod diameter</th>
<th>Pellet diameter</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{233}\text{UO}_2$-$\text{ZrO}_2$ seed</td>
<td>24.47</td>
<td>23.81</td>
<td>0.6477 cm (0.255 in.)</td>
<td>0.53594 cm (0.211 in.)</td>
</tr>
<tr>
<td>$^{235}\text{UO}_2$-$\text{ZrO}_2$ seed</td>
<td>24.70</td>
<td>22.90</td>
<td>0.6477 cm (0.255 in.)</td>
<td>0.53594 cm (0.211 in.)</td>
</tr>
<tr>
<td>$^{235}\text{UO}_2$-$\text{ThO}_2$ blanket</td>
<td>0.939</td>
<td>0.913</td>
<td>1.44526 cm (0.569 in.)</td>
<td>1.24446 cm (0.490 in.)</td>
</tr>
<tr>
<td>ThO$_2$ blanket</td>
<td>NA</td>
<td>NA</td>
<td>1.4478 cm (0.570 in.)</td>
<td>1.24206 cm (0.489 in.)</td>
</tr>
</tbody>
</table>

Table 5.6: Information on fuel matrices. Note that the clad thicknesses were 0.04445 cm and 0.09017 cm in the seed and blanket rods respectively.
The benchmark model consisted of a cylindrical water reflector that extended 30.48 cm (12 in.) above and below the fuel rods and at least 30.48 cm beyond the outermost fuel rod. This was because beyond around 30 cm neutrons in light water are unlikely to return to the system and therefore it is unnecessary to model detail further than 30 cm. The benchmark model also ignored grid spacers, support plates and trace nuclides within the U and Th fuels and the Zr-based clad material. The overall effect of such simplifications resulted in a bias of up to -0.0020 [183]. The results from the MONK calculations are detailed in Table 5.7.

From Table 5.7 it can be seen that whilst none of the discrepancies associated with the JEFF 3.1 results are greater than 1% there were a large number of discrepancies greater than 2 \( \sigma \). This was inconsistent with the results from the previous sets of experiments where the general trend was for smaller discrepancies using JEFF 3.1 nuclear data libraries compared to JEF 2.2. Therefore, attention focuses here on the primary differences between the experiments modelled in the earlier sections and the seed and blanket core experiments. A major difference is that large concentrations of zirconium and oxygen are present within the reactive seed regions and these are not present in any of the experiments modelled earlier in this chapter.

A significant difference between JEFF 3.1 and subsequent versions of the JEFF nuclear data library, that is relevant to the cores studied in this section, is that using JEFF 3.1 tends to overestimate absorption by the Zr and O elements, in particular the 292.41 eV resonance for \(^{91}\text{Zr}\) and the \((n,\alpha)\) reactions below 6.0 MeV for \(^{16}\text{O}\) [185]. This would explain why the MONK \(k_C\) results were always less than the benchmark \(k_{eff}\) results and hence the negative discrepancy values for the JEFF 3.1 results shown in Table 5.7. Therefore, the models were re-run replacing the zirconium and oxygen data libraries with their JEFF 3.1.2 equivalents.

The JEFF 3.1/JEFF 3.1.2 results shown in Table 5.7 exhibited in general smaller discrepancies and significantly fewer discrepancies greater than 2 \( \sigma \) when using the JEFF 3.1.2 data library for zirconium and oxygen relative to using solely JEFF 3.1 for all nuclides present within the system.

### 5.5 Discussion and Conclusion

Tables 5.8 and 5.9 summarise the results from the \(^{232}\text{Th}\) and \(^{233}\text{U}\) experiments respectively, where in the case of the light water breeder blanket experiments the cores that contain \(^{233}\text{U}\) in the seed region have been designated \(^{233}\text{U}\) cores and the remainder designated \(^{232}\text{Th}\) cores.
<table>
<thead>
<tr>
<th>Core ID</th>
<th>H:HM in seed</th>
<th>H:HM in blanket</th>
<th>JEF 2.2 (%)</th>
<th>JEFF 3.1 (%)</th>
<th>JEFF 3.1/JEFF 3.1.2 (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SB-1</td>
<td>37</td>
<td>4.4</td>
<td>0.18 ± 0.27</td>
<td>-0.67 ± 0.27</td>
<td>-0.54 ± 0.27</td>
</tr>
<tr>
<td>SB-2</td>
<td>39</td>
<td>4.4</td>
<td>0.83 ± 0.25</td>
<td>-0.39 ± 0.25</td>
<td>-0.37 ± 0.25</td>
</tr>
<tr>
<td>SB-2.5</td>
<td>39</td>
<td>NA</td>
<td>1.20 ± 0.25</td>
<td>-0.31 ± 0.25</td>
<td>-0.34 ± 0.25</td>
</tr>
<tr>
<td>SB-3</td>
<td>39</td>
<td>4.4</td>
<td>0.22 ± 0.25</td>
<td>-0.74 ± 0.25</td>
<td>-0.65 ± 0.25</td>
</tr>
<tr>
<td>SB-4</td>
<td>37</td>
<td>4.4</td>
<td>-0.20 ± 0.26</td>
<td>-0.72 ± 0.26</td>
<td>-0.63 ± 0.26</td>
</tr>
<tr>
<td>SB-5</td>
<td>110</td>
<td>0.45</td>
<td>-0.68 ± 0.28</td>
<td>-0.88 ± 0.28</td>
<td>-0.48 ± 0.28</td>
</tr>
<tr>
<td>SB-6</td>
<td>110</td>
<td>0.45</td>
<td>0.27 ± 0.27</td>
<td>-0.55 ± 0.27</td>
<td>-0.17 ± 0.27</td>
</tr>
<tr>
<td>SB-7</td>
<td>110</td>
<td>0.45</td>
<td>-0.33 ± 0.28</td>
<td>-0.90 ± 0.28</td>
<td>-0.55 ± 0.28</td>
</tr>
</tbody>
</table>

Table 5.7: Discrepancies from using BINGO JEF 2.2 and BINGO JEFF 3.1 libraries. The cells highlighted in yellow correspond to discrepancies greater than 2σ between the $k_C$ and $k_B$. Red and blue cells correspond to experiments where the predominant fissile nuclides were $^{235}\text{U}$ and $^{233}\text{U}$ respectively.
Table 5.8: Summary of the discrepancies between the benchmark results and MONK using the JEF/F nuclear data libraries for cores containing $^{232}\text{Th}$.

<table>
<thead>
<tr>
<th>Nuclear Data Library</th>
<th>Proportion of results that are:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$&lt; 0.5%$</td>
</tr>
<tr>
<td>JEF 2.2</td>
<td>45%</td>
</tr>
<tr>
<td>JEFF 3.1</td>
<td>52%</td>
</tr>
</tbody>
</table>

Table 5.9: Summary of the discrepancies between the benchmark results and MONK using the JEF/F nuclear data libraries for cores containing $^{233}\text{U}$.

<table>
<thead>
<tr>
<th>Nuclear Data Library</th>
<th>Proportion of results that are:</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$&lt; 0.5%$</td>
</tr>
<tr>
<td>JEF 2.2</td>
<td>36%</td>
</tr>
<tr>
<td>JEFF 3.1</td>
<td>73%</td>
</tr>
</tbody>
</table>

Table 5.8 indicates that in the case of the thorium experiments where the predominant fissile nuclide was $^{235}\text{U}$, the results from MONK are broadly the same independent of whether the JEF 2.2 or JEFF 3.1 data libraries are employed. The majority of cases have discrepancies less than 1%, although only around half of the cases give good agreement ($< 0.5\%$) with the expected benchmark value. On the other hand, there is a considerable difference between the JEF 2.2 and JEFF 3.1 nuclear data libraries for the $^{233}\text{U}$ experiments, with JEFF 3.1 results showing in general smaller discrepancies between the MONK calculated value and the benchmark value. However, by combining the results together from the four very different sets of experiments the individual discrepancy behaviour from each set of experiments has been lost, namely:

- The seed and blanket experiments just so happened to contain significant quantities of materials (O and Zr) where deficiencies in the JEFF 3.1 nuclear data library are known to exist. If these were excluded from the summary table then the proportion of JEFF 3.1 showing discrepancies less than 0.5% would increase to 82% and for the case of JEF 2.2 results would decrease to 29%.

- The majority of the $^{233}\text{U}$ discrepant results come from the uranyl nitrate experiments that had relatively high H:HM ratios (> 100) in comparison to the Thorium Uranium Physics Experiment results and the seed/blanket experiments.

- The majority of the $^{232}\text{Th}$ results also came from a single set of experiments that had relatively low H:HM ratios (< 15).

The general behaviour in most sets of experiments was that as the spectrum hardened (H:HM
reduced) the discrepancy tended to increase. This behaviour is shown by the fact that:

- The discrepancy tended to increase for both JEF/F libraries in the Thorium Uranium Physics Experiments (TUPE), see Figures 5.8 and 5.9.

- The RBMK experiments showed larger discrepancies for the unflooded cases relative to the flooded cases for both JEF/F libraries, see Figures 5.12 and 5.13. Note that cores with light water tend to exhibit a more thermalised spectrum relative to graphite moderated systems as hydrogen readily slows down neutrons relative to carbon (around 14 and 90 elastic collisions are required to reduce neutron energies from 2 MeV to 1 eV in the case of hydrogen and carbon moderators respectively [167]). Therefore it is reasonable to expect a significantly softer spectrum in the flooded RBMK cases relative to the unflooded cases.

The dependence of discrepancy on low H:HM values probably explains why the $^{232}$Th results for both JEF/F libraries have only around half of the results showing good agreement between MONK and the expected benchmark values. This is because all of the TUPE systems had relatively low H:HM values. The reason for worsening discrepancy performance as a function of H:HM is likely due to the fact that absorption cross-sections in cores with low H:HM values will be more dependent on resonance absorptions. Resonance absorption is characterised by large deviations in absorption cross-sections over relatively small flux intervals that are determined primarily by experiments. Therefore, the resonance region is more prone to experimental uncertainty. In comparison at low neutron energies there is considerably less sensitivity to small changes in flux and the absorption cross-sections can readily be approximated by a $1/v$ dependence [15].

In conclusion, for systems that contain limited $^{233}$U and/or considerable $^{232}$Th there is limited difference in the performance between JEF 2.2 and JEFF 3.1 and both exhibiting larger discrepancies in systems with low H:HM ratios. However, in the case where significant inventories of $^{233}$U exist then JEFF 3.1 has been shown (see Table 5.9) to exhibit considerably lower discrepancies for a variety of experiments. Therefore in the case of systems such as the (Th,U)O$_2$ marine core designed in this study, where the predominant nuclides are Th, $^{235}$U and $^{238}$U, there is likely to be little benefit utilising JEFF 3.1 relative to JEF 2.2. However, in the case for cores that contain large proportions of $^{233}$U, such as light water and heavy water breeder reactors operating on a $^{232}$Th-$^{233}$U cycle, it is recommend that JEFF 3.1 and later versions are utilised.
Chapter 6

Conclusion

Two small reactor cores have been designed, one containing UO$_2$ fuel and the other (Th,U)O$_2$ fuel. Both designs have achieved the majority of goals and requirements set out in Chapter 2:

- $^{235}$U concentrations less than 20 wt.%;
- Power outputs of 411.4 MWth over a 15 year core life;
- No soluble boron during operation;
- Cores fit within a 3.5 m Reactor Pressure Vessel (RPV).

Whilst conventional light water technology has been employed, in other words using UO$_2$ fuel within cylindrical tubes of zirconium-based alloy, the current core design requires future modification in order to ensure:

- Peak clad surface temperature $< 310^\circ$C;
- Maximum clad hoop creep throughout life $< 1$%;
- Maximum rod internal pressure throughout life $< 15.5$ MPa.

Investigations in Chapter 3 have shown that, for the UO$_2$ core design, relatively small modifications (in particular increasing the pellet-clad gap size from $8.2 \times 10^{-3}$ cm to around $2 \times 10^{-2}$ cm) are required in order to ensure the rod internal pressure and maximum clad hoop creep strain meet their criteria. This is especially true if future core designs limit the maximum rod burnup to less than 100 GW.d/tHM.
6.1 Issues Regarding Core Parameters

Now that the core has been designed it is possible to discuss in detail what issues have been raised regarding some of the parameters in Chapter 2; in particular key issues regarding the soluble boron free goal, fuel assembly geometry and the imposed criterion regarding a single rod geometry used throughout the entire core.

6.1.1 Soluble Boron Free Design

Soluble boron in conventional PWRs functions as both a means to control reactivity during power operation and an important safety system that is able to achieve large shutdown margins in any reactor state. However, total elimination was found to be highly beneficial (see Section 2.6 in Chapter 2) assuming its role as an important safety system could be replicated by some other system. An alternative system would be to utilise two different (diverse) Control Rod Drive Mechanisms (CRDMs), with each set of CRDMs able to insert sufficient Rod Control Cluster Assemblies to meet the required shutdown margins (redundancy). The advantage of this method would be the elimination of the need for soluble boron. In addition, control rods are able to achieve shutdown far quicker than soluble poison (see Section 2.6 in Chapter 2). However, in Chapter 3 it was found that it would require all assemblies to have an RCCA present to ensure that in the event the highest worth RCCA is removed there was sufficient remaining rod worth to ensure shutdown margins were met. This implies that it may prove difficult to implement such a strategy as no single set of CRDMs/RCCAs would be able to achieve adequate shutdown margins if the other set failed. Furthermore, in the event of fuel melting and relocation occurring, the usefulness of mechanical shutdown becomes limited as the melted fuel could be in a location within the core where the control rods do not interact. An advantage of soluble poison is that as long as the core is flooded with a sufficient concentration of soluble poison then relocation of fuel is much less of a concern.

It may be possible to create a fuel design that inherently limits reactivity once melting has occurred, or to incorporate sacrificial material within the core that - when coming into contact with molten fuel - will interact and absorb neutrons. Section 6.4.1 discusses some potential strategies to achieve this; however, such strategies are complicated by the fact that any density differences within the molten fuel mixtures can lead to separation through buoyancy effects [186]. Hence, if the neutron absorbing material starts to separate from the fissile components within the molten mixture, re-criticality may
arise. It therefore seems sensible to assume that soluble boron will be required for certain accident conditions. However, advantages still remain relative to a system that uses soluble boron during normal operation as this (see Section 2.6 in Chapter 2 for further details):

- Reduces the risk of boron-induced corrosion;
- Simplifies coolant chemistry, thereby reducing the required sampling and also allows for considerable simplifications of the Chemical and Volume Control System;
- Reduces the overall likelihood of inadvertent boron dilution occurring as the vast majority of time no boron will be present within the reactor coolant;
- Improves safety as two truly redundant and diverse reactivity control mechanisms are present.\(^1\)

However, as there is the possibility that the reactor coolant may contain boron during some accident events this results in the following disadvantages:

- Extra systems will need to be in place to remove boron once it has entered the coolant or it is assumed that the ship will operate under auxiliary power and return to a port where these facilities are available;
- Limitations will be in place with respect to what water reservoir can be utilised to ensure sufficient core cooling, for example, in the event that the reactor coolant is borated, but further coolant is required, then it will not be possible to inject water from a reservoir that contains no soluble boron;
- Any pipes that may carry borated water will require heating to ensure blockages resulting from precipitation do not occur, resulting in increased complexity.

### 6.1.2 Fuel Assembly and Rod Geometry

The chosen 17 by 17 square assembly design was appropriate assuming that future optimisation work is able to limit peak rod burnup to below 100 GW.d/tHM. If not then it would be sensible to look into alternative assembly designs that allow for a greater number of rods to be inserted into the reactor.

\(^1\)In conventional PWRs there are periods of time where the control rod worth is not sufficient alone to ensure adequate shutdown margins, without the additional use of soluble boron.
pressure vessel. This would reduce the power of each rod and also reduce the peak rod burnup. Alternative fuel assembly designs are discussed in Section 6.4.

The limitation imposed by insisting on a single rod geometry throughout the core (fixed plenum length, pellet-clad gap and pellet dimensions) is in hindsight too restrictive. This is due to the fact that this core does not employ any fuel shuffling; it is very infrequently refuelled and it suffers from relatively high local power peaking factors. It would be sensible therefore to remove this limitation and allow optimisation by tailoring rod geometry to the power history the rods operate under. Whilst more fuel rod types will increase manufacturing complexity there are benefits to improving flexibility. For instance, by allowing rods to be optimised for their particular locations this would permit the following:

- Reduce unnecessarily large plenum sizes for low burnup rods, which will result in reduced material requirements;
- Optimising channel mass flow rates to improve thermal-hydraulic performance as lower power rods will have lower channel outlet temperatures relative to higher power rods for a fixed channel mass flow rate. This will result in cooler water mixing with hotter water at the top of the core reducing coolant outlet temperature, thereby creating a thermal efficiency penalty. By altering rod sizes within certain regions of the core it may be possible to improve the thermal efficiency. In addition, this permits the hotter rods to have higher mass flow rates to ensure the peak clad surface temperature is below 310°C.

It would also be worth investigating the use of channel boxes to alter mass flow rates across the core in addition to altering fuel rod diameters. Furthermore, whilst employing a greater variety of rod geometries will have a negative effect on manufacturing costs, it is worth noting that commercial BWRs have considerably more complicated assembly designs (utilising a variety of enrichment and rod geometries within a single assembly [187]). Hence more complexity is not commercially prohibitive.

### 6.2 Issues Regarding the Modelling of Long-Life Cores

#### Neutronics

Insisting the core has a very long core life whilst limiting the quantity of fuel within the reactor pressure vessel, and also removing soluble boron, has meant that the enrichment and poison concentration are
much higher than in conventional PWRs. Hence the increased proportion of nuclides with high thermal absorption cross-sections ($^{235}\text{U}$, $^{155}\text{Gd}$ and $^{157}\text{Gd}$) has resulted in the core becoming an epithermal system at the beginning of life. By modelling the $\text{UO}_2$ marine core design in MONK and CASMO-SIMULATE it was found that significant discrepancies arose between the two codes utilising the same nuclear data library (JEF 2.2). This is because of the following:

- Inadequate energy group structure (size and number of energy groups) in CASMO for modelling epithermal spectra;
- The assumption of a thermal flux used to produce the multi-group constants in CASMO.

A similar, albeit more pronounced, effect was observed in the ($\text{Th, U}) \text{O}_2$ CASMO cases. This is likely to be because, whilst the discrepancy is relatively large for epithermal $\text{UO}_2$ systems, some optimisation in selecting the energy group structure for $^{235}\text{U}$ and $^{238}\text{U}$ has been performed. However, much less optimisation has been performed regarding the required group structure for $^{232}\text{Th}$.

Furthermore, a variety of $^{232}\text{Th}$ and $^{233}\text{U}$ experiments were performed to assess the suitability of JEF 2.2 for modelling such systems. It was found that JEF 2.2 gave relatively large discrepancies for systems containing $^{233}\text{U}$ relative to the newer JEFF 3.1 library, although the performance of the JEF 2.2 library for $^{232}\text{Th}$ was comparable to the JEFF 3.1 library.

**Fuel Performance**

The main issue in the long-life core design was that the peak rod burnup within the core was much higher than in modern PWRs. In addition, by operating the core without soluble boron, the peak rod burnup is further increased as power peaking is more pronounced. Hence the peak rod burnup in the marine core design was around 120 GW.d/tHM compared with typical peak burnups of around 60 GW.d/tHM in modern PWRs. Beyond around 100 GW.d/tHM the necessary fuel performance data such as thermal conductivity degradation and fission gas release becomes sparse. This further adds weight to requiring future core iteration to keep peak rod burnups below 100 GW.d/tHM.

### 6.3 Benefits of ($\text{Th, U}) \text{O}_2$ Fuel over $\text{UO}_2$ Fuel

In the case of the ($\text{Th, U}) \text{O}_2$ core the fuel performance relative to $\text{UO}_2$ fuel was shown to be inferior even though it is generally stated [164, 18, 165] that thorium-based fuels exhibit considerably improved
thermo-mechanical behaviour. The reason behind the inferiority of (Th,U)O$_2$ fuels in this novel core design was in part due to the relatively low power density inherent in achieving its long core life. By operating at lower power densities the fuel temperatures were on average much lower than in modern PWRs. This resulted in the thermal conductivity, $\lambda(T)$, for (Th,U)O$_2$ exhibiting lower thermal conductivities relative to UO$_2$ operating under the same power histories, see Figure 4.19.

For (Th,U)O$_2$ fuel to be judged better than UO$_2$ fuel it would be necessary for (Th,U)O$_2$ fuel to show significant improvements in the following characteristics:

- Whilst it is known [34] that thorium-based fuels exhibit lower creep rates, the precise dependence of creep rates as a function of uranium content is currently unknown. ENIGMA assumes the creep rate for (Th,U)O$_2$ is the same as ThO$_2$ fuel, which is much lower than UO$_2$ fuel, and therefore the fuel is unable to relieve stress within the system by deforming. Hence stress accumulates in the clad. It would therefore be necessary for (Th,U)O$_2$ fuel to show similar creep rates to those of UO$_2$ fuel for most U contents in order to diminish this assumed detrimental creep characteristic for thorium-based fuel.

- There is currently uncertainty with regards to the diffusion coefficient for (Th,U)O$_2$ fuels as a function of temperature below approximately 1400 K. ENIGMA effectively assumes that the diffusion coefficient of (Th,U)O$_2$ fuel at temperatures below around 1400 K is the same as UO$_2$ fuel. Therefore, to significantly reduce fission gas release, the $D_{\text{mix}}$ and/or $D_{\text{ath}}$ will need to become much smaller to compensate for the inferior thermal conductivity of (Th,U)O$_2$ fuel at low temperatures.

The main benefit of utilising (Th,U)O$_2$ was the lower Gd$_2$O$_3$ concentrations. However, due to lack of data on (Th,U,Gd)O$_2$ fuel types it was not possible to perform a comparison with the equivalent UO$_2$ fuel. This further highlights the fact that in general the sparse data on (Th,U)O$_2$ makes detailed fuel performance comparisons with UO$_2$ difficult. Furthermore, given that no net benefit was found in the economic performance of the two reactor designs with both having similar fuel costs, we suggest that future work focuses on improving the UO$_2$ core design. However, if data becomes available that shows significant improvements regarding creep and fission gas release for (Th,U)O$_2$ fuel, in addition to significant benefits attached to the lower Gd$_2$O$_3$ concentrations required in the (Th,U)O$_2$ design, then it may become preferable to develop the (Th,U)O$_2$ core further.
6.4 Future Work

There is scope to improve the fuel performance characteristics of this core by utilising an improved optimisation method (discussed below). This is because currently the peak rod burnup in both (Th,U)O$_2$ and UO$_2$ cores is very high ($\sim 120$ GW.d/tHM). These burnups are beyond the validation database for fuel performance codes such as ENIGMA resulting in the need to extrapolate the performance characteristics for UO$_2$ fuel. By reducing the peak rod burnup to below 100 GW.d/tHM not only does this result in only relatively small alterations in fuel rod geometry (e.g. it is not necessary to implement annular pellets, which further raises rod burnup, in order to reduce rod internal pressure) but it results in rod burnups that are within ENIGMA’s validation database. Furthermore, data has been found \[39\] on UO$_2$ fuel operating up to 98 GW.d/tHM under similar conditions (low power densities, ultra-high burnups and within a PWR) to the fuel rods within this study. Hence, it is suggested that future work focuses on ensuring peak rod burnups are below 100 GW.d/tHM.

Related to the performance of fuel is the survivability of the clad material over core life. To achieve the chosen 15 year core life it was necessary to significantly reduce peak clad temperatures from the 350°C that modern PWR fuel achieves, to 310°C. The peak clad coolant temperature of 310°C was based on the results from the corrosion performance of CANDU Pressure Tubes (PTs) and comparing the Zr-2.5Nb alloy used in PTs with 2nd generation PWR clad materials (namely ZIRLO). However, this comparison was based on the materials exposed to pure (likely stagnant) high-temperature water which is not necessarily reflective of in-reactor corrosion rates because of the effects of heat, neutron flux and the precise chemical conditions. As CANDU reactors do not employ soluble poison within the PTs it was assumed that the chemical conditions for the fuel rods within the reactor designed in this study would be similar to CANDU water chemistry, i.e. pH within the range 10-10.2 \[106\]. It is suggested that work should be performed to assess advanced Zr-based alloys (for example ZIRLO, M5, E110, AXIOM and Areva’s ‘Q’ alloys) under CANDU water chemistry conditions. In addition, given the high stresses the cladding material must withstand, due to the swelling of high burnup fuel, it is important to also assess the advanced Zr-based alloys in terms of their strength. This information could then be used to select the preferred alloy for testing within reactor-like conditions (i.e. neutron and gamma irradiation along with temperature gradients along the fuel rod) to test the likelihood of clad survivability.

It was decided in Chapter 2 that a single rod geometry would be studied to reduce manufacturing
costs and also to lessen the number of variables within the reactor design. However, as discussed earlier, the limitation imposed by insisting on a single rod geometry is in hindsight too restrictive. Hence in future work it would be sensible to remove this limitation to allow further fuel optimisation. It would also be worth investigating the use of channel boxes to alter mass flow rates in addition to altering fuel rod diameters to control coolant flow rates across the core.

### 6.4.1 Alternative Poison Choices

Gadolinium was the preferred poison; however, there may be benefits in alternative poisons. In particular due to the long core life and rapid depletion of gadolinium it was necessary to incorporate up to 20 wt.% gadolinia within the fuel. This will have detrimental impacts on fuel conductivity (see Appendix B.1), and there is limited experience with such poison concentrations. The use of enriched gadolinium could help reduce the performance degradation that occurs with high gadolinia concentrations, namely the deterioration of fuel thermal conductivity. In addition, the uncertainty surrounding gadolinia concentrations above 15 wt.% could be avoided if enriched gadolinia permits a reduction in the gadolinia concentration. However, as gadolinia concentration is reduced, the fissile density will increase, which may result in significant power peaking towards the end of life (EOL). This could be offset by varying the enrichment in these pins (which was ignored as the gadolinia concentration was relatively high in all BPPs, thereby reducing the effective fissile density of BPPs).

Potential poison options that should be studied besides gadolinium are those listed in Chapter 2 which were: europium, hafnium, dysprosium and erbium. However, for all of these poisons, besides erbium, there is limited material information\(^2\). It would therefore be sensible to investigate lattice configurations for these poisons with regards to achieving the targeted 15 year core life. Then the best performing poisons (with respect to reactivity suppression with minimum poison concentrations) should have their fuel performance properties assessed, in particular: thermal conductivities as a function of temperature; achievable fuel densities through conventional sintering processes; and mechanical properties including elastic modulus and creep rates.

Hybrid poisons may also offer superior behaviour in comparison to a single mixture of either poison. For instance by mixing gadolinium with a poison that depletes relatively slowly, such as erbium or hafnium, it may be possible to suppress initial reactivity whilst minimising the reactivity swing without high concentrations of burnable poison.

\(^2\)(U,Er)\(_2\)O\(_3\) is also known to suffer from low achievable fuel densities with high Er\(_2\)O\(_3\) concentrations [137].
A key question related to the feasibility of total elimination of soluble boron is whether it would be possible to ensure with sufficient confidence that even in the most severe accidents (i.e. core melt has occurred) an acceptable sub-criticality margin can be achieved only using unborated water. Two ways to achieve this would be: 1) the addition of sacrificial material to the inside of the RPV that would interact with any molten fuel and ensure sufficient sub-criticality in the presence of unborated water [188] and/or 2) the burnable poisons used have the characteristic that upon melting their poison worth increases to such an extent that in any likely core configuration $k_{eff}$ is below 0.95. The modelling of these scenarios would have to include any buoyancy effects of the different materials, for instance uranium is likely to separate from the lighter burnable poisons and zirconium within the fuel [186]. Therefore it may be possible that with sufficiently robust control rods, coupled with the fact that even in the event of core melt it is still possible to achieve a sufficiently low sub-criticality margin, total elimination could be achieved.

The use of an alternative poison configuration to the one employed in the marine core design may allow option 2) to be achieved. For instance, we propose a micro-heterogeneous fuel that includes thin discs of burnable poison sandwiched between fuel pellets. The disc material should have a melting temperature comparable to the temperature at which fuel melting occurs. Furthermore, the disc material should have the property that, when it starts to become a homogeneous mixture with the molten fuel, its poison worth increases. The disc material should also burn out relatively slowly to ensure that it has sufficient negative reactivity towards the end of life that it is still capable of reducing the reactivity of the fuel upon melting. However, the disadvantage is that the residual poison penalty will be higher. A further disadvantage is that such a micro-heterogeneous concept would also complicate fuel manufacturing as more components are required in constructing fuel rods.

Materials based on europium, erbium, hafnium, dysprosium and erbium may be able to achieve the above requirements. Finally, if the material were found to have superior thermal conductivity relative to $\text{UO}_2$ fuel then this would improve heat transfer between the pellet and the clad.

6.4.2 Improved Optimisation

The current optimisation process, in particular the automated search process, is inefficient with respect to the computational cost in determining viable core designs (of the 9216 cores constructed only around 2% met the criteria regarding maximum control rod insertion and maintaining sufficient reactivity over the 15 year core life). The main reason for this inefficiency is that the discriminator algorithm
in its current form is incapable of focusing computational effort on the cores with more favourable characteristics. For example, cores with top and bottom axial regions of 80 cm and 20 cm respectively generally have smaller local peaking factors and shallower control rod insertion. By comparison, cases with top and bottom regions of 60 cm and 1 cm generally give poorer results. It is therefore inefficient to continuously dedicate equal amounts of computation time to assessing both cases. The same reasoning is also true for enrichment and burnable poison concentrations within regions of the core as some combination of these two characteristics will result in too much reactivity or too little reactivity over core life, necessitating deep control rod insertions or reductions in core life respectively. Hence, an optimisation process that counteracts these problems is required.

Stochastic optimisation algorithms have been utilised in reactor design as they focus computation on cases with more favourable characteristics. For example so-called genetic algorithms, which focus computation on the most favourable cases (individuals), have been successfully employed in optimising core loading patterns [189, 190, 191]. Genetic algorithms mimic the process of natural selection by taking a series of individuals (in this case reactor cores) and allowing the key (genetic) information (this could be loading pattern layout, enrichment zoning, control rod layout, etc.) of the best performing individuals to combine (mate) and transfer these characteristics to the next generation. Subsequent generations should therefore contain individuals with better characteristics relative to the previous generation, eventually resulting in an optimal solution to the problem. However, to speed up the process of finding an optimal solution it is essential to put in place criteria that are known to generally result in favourable characteristics. The work set out in Chapters 3 and 4 can be used to form these criteria.

As was the case with the method employed throughout this investigation to create viable core designs, the task could be split into three processes:

1. Construct lattices to be implemented into a 3D core model;
2. Radially optimise the finite 3D core layout;
3. Axially optimise the finite 3D core with control rods present.

Each of the three items listed above could likely be improved, resulting in a core design that has significantly lower local peaking factor throughout life and a reduced peak rod burnup.

The improved core could then be assessed in terms of transient performance, especially with respect
to determining whether or not ejection of the highest worth rod will result in fuel failure. The results from this study could be used to alter limits on RCCA penetration during power operation.

Once a core with an improved power distribution over time is created, the core could then be assessed with respect to fuel performance and thermal-hydraulics. If it is still the case that any of the criteria relating to clad surface temperature, maximum rod internal pressure and/or maximum clad hoop creep strain are not met then further alterations to fuel rod geometries could be made. This could include adjusting the channel flow rates by altering rod dimensions and/or incorporating channel boxes to alter flow rates within certain assemblies.

If none of the above is able to achieve satisfactory thermal-hydraulic and fuel performance criteria then the adoption of smaller assemblies using thinner rods should be assessed. This would permit a significant increase in the number of rods residing in the core thereby reducing the maximum power and burnup any single rod is exposed to.

The development of an entirely new assembly design is probably best avoided due to the issues raised in Section 3.3.1 in Chapter 3. Furthermore, given the preference for a smaller RPV, an assembly that is smaller and better approximates a circle would be justified, i.e. hexagonal assemblies. The VVER-440 reactor is one of the few PWRs to utilise hexagonal assemblies and has been employed on a large scale for a number of decades [16]. The VVER-440 used assemblies with a pitch of 15.99 cm (vs 21.42 cm for the assembly used in this study) that contain 127 rods each [192]. Hence VVER-440 assemblies typically contain around 35% more fuel rods per unit area than typical (17 by 17) PWR assemblies [192]. However, as each rod is thinner than typical PWR rods, then for the same active fuel length (and assuming non-annular pellets in both cases) this results in around 15% less fuel per fuel rod. Overall, an increase in the fuel heavy metal mass of around 20% should be possible with a resulting decrease in peak core burnup. In addition, the power output from each rod would significantly decrease resulting in lower clad surface temperatures, thereby reducing the extent of corrosion. The disadvantage of this strategy is that the greater number of fuel rods within the core will have an associated increase in cost due to the greater number of fuel rods to manufacture.

6.4.3 Design Basis Accidents

When analysing the safety performance of a reactor design it is typical to analyse the system against a variety of postulated failures [167]. The most demanding of these postulated failure scenarios are termed Design Basis Accidents (DBAs). DBA analysis forms part of the routine assessment when
licensing a reactor design. Therefore of most interest here is where marine reactor accidents would differ from their land-based counterparts.

<table>
<thead>
<tr>
<th>Accident Category</th>
<th>Accident Frequency (per ship year)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Collision</td>
<td>$7.04 \times 10^{-3}$</td>
</tr>
<tr>
<td>Grounding</td>
<td>$4.70 \times 10^{-3}$</td>
</tr>
<tr>
<td>Fire/explosion</td>
<td>$1.95 \times 10^{-3}$</td>
</tr>
<tr>
<td>Foundering</td>
<td>$1.2 \times 10^{-4}$</td>
</tr>
<tr>
<td><strong>Total</strong></td>
<td>$1.38 \times 10^{-2}$</td>
</tr>
</tbody>
</table>

Table 6.1: The frequency of certain accidents in the container ship fleet from the year 1990 to 2012 [23].

Table 6.1 shows the accident frequencies per ship year for container ships in the period 1990 to 2012, categorised by accident type. Taking into account that in nuclear safety incidents with a frequency of $10^{-3}$ or higher are considered frequent faults, it is difficult to see how any of the above categories would not make up part of the safety assessment. However, Table 6.1 does not discuss the severity of any of the incidents, for example do all fires/explosions result in damage to the integrity of the hull or necessitate external assistance? Furthermore, there are no details on the likelihood of an accident occurring based on the age of the ship, for instance are newer larger container vessels more or less likely to experience to certain accidents?

It is worth considering each of the categories outlined in Table 6.1. First, it would be expected that in a nuclear powered ship (with perhaps a few small diesel generators for auxiliary power) the amount of flammable liquid fuel on board the ship would be considerably reduced in comparison to conventional diesel powered ships. This may therefore significantly reduce the likelihood of fires/explosions occurring. Besides explosions caused by, for example, certain cargo or the detonation of combustible material, there is also willful human interference. For instance, it is plausible that a group of individuals may want to load a small vessel up with explosives and target the side of a nuclear powered ship in order to cause panic. The key concern therefore is the likelihood of the nuclear containment vessel failing. However, as containment vessels must be able to cope with large amounts of energy generated within the reactor core and therefore are very robust, it may be the case that the containment vessel is able to cope with such a scenario [193, 194]. Therefore, it may be possible to render such scenarios of limited concern.

Foundering (the sinking of a ship due to taking on board water) is also a category that does have some precedent, as a number of nuclear powered vessels have been sunk [56, 195]. However, in all
of the cases reported the reactor was successfully shut down (and remained so) [195]. In addition, it appears that given the high-integrity materials used for constructing nuclear reactors, the nuclear fuel has not been openly exposed to seawater. All of these have resulted in relatively limited exposure to radionuclides [195]. In addition, it is certainly the case that concerns are more likely to be raised if a ship sinks in relatively shallow water near a populated area, and hence retrieval of the core may be necessary. But even here there is experience relating to the retrieval of once-active nuclear cores from the seabed [195]. Therefore foundering may be less of an issue than the occurrence frequency implies.

Even if fires/explosions and foundering are not considered prohibitive barriers to the deployment of marine reactors in civilian settings it is difficult to see how collision and grounding would not constitute design basis accidents. In the case of collision, it would be necessary to calculate the likely stresses during the collision between two vessels travelling at typical port speeds (where collisions are more likely) that would be imparted on the containment vessel of the nuclear ship. It may be possible to ensure that the likelihood of containment failure is sufficiently low by utilising active systems that can detect any sudden impact and therefore shut down the core, along with the addition of systems to absorb and counteract the shock [196]. This could permit the containment vessel to operate within its design constraints. However, without at least performing the necessary calculations it is not possible to rule out the use of nuclear powered ships on accident frequencies alone.

With respect to grounding (defined as the impact of a shipping vessel with the seabed) this, along with collisions, is likely to constitute the worst of the accidents featured in Table 6.1. This is because a grounding accident could result in the loss of the ultimate heat sink (the sea), for example getting caught on the seabed followed by the tide going out. This could result in major damage to the core unless systems are in place to overcome such a situation, for example a large reservoir on board the vessel with sufficient coolant inventory to cool the reactor core until help arrives.

Assuming appropriate safety measures are in place regarding collision and grounding accidents then there does not appear to be any reason in principle why a nuclear powered ship cannot operate safely. However, it may be the case that the countermeasures necessary to reduce the probability of radionuclide release result in the reactor design becoming uneconomic relative to fossil fuelled cargo vessels that are currently able to release their waste to the atmosphere with no economic penalty.
6.4.4 Graphite Moderated, Gas-Cooled Reactor

Graphite moderator, gas-cooled reactors might be an alternative to LWRs for marine propulsion. A significant advantage of graphite moderated, gas-cooled reactors over light water reactors is their generally high levels of passive safety. However, their inherent low power density (due to carbon’s relatively poor ability to slow down neutrons in a single collision thereby necessitating a larger volume of moderator) in addition to the poor heat transfer properties of the coolant relative to water makes them generally more expensive than LWRs. In addition, the use of a complex ceramic fuel further increases costs [167]. Finally, their low power density, and thus large size for a given power output, may result in a reactor design that is prohibitively large, even when factoring in the potential for a smaller/simpler containment structure. Therefore, the suitability of deploying LWRs for marine propulsion should take preference in terms of studying their suitability and performance, with the gas-cooled, graphite moderated concept as a potential second option if prohibitive barriers are found in deploying LWRs from a safety perspective.

6.4.5 Future Work Summary

Unless data becomes available showing significant improvement in (Th,U)O$_2$ fuel creep rates, $D_{\text{mix}}$ and $D_{\text{ath}}$ diffusion coefficients and the thermal conductivity of (Th,U,Gd)O$_2$ fuel relative to (U,Gd)O$_2$ fuel then there is no net benefit regarding the deployment of (Th,U)O$_2$ fuel in the long-life core designed in this study. Therefore it is recommended that future work focuses on improving the UO$_2$ core design and addressing limitations in this study. Hence, future work is split into primary, secondary and other potential considerations, which represent where future work should be focused. Primary work is mainly focused on addressing uncertainties with respect to the ability of codes to accurately predict the neutronic and fuel performance behaviour of the fuel utilised in the core designed in this study, along with areas the author thinks could permit significant improvements in the final core design. Secondary work is predominantly based on areas that may allow for further improvements in the final core characteristics and areas that must be eventually addressed to permit licensing of a long-life core. Finally, other potential considerations are mainly areas of work that can be used to permit a comparative assessment between different core designs.
Primary

• Future cores should utilise fuel rods with a larger pellet-clad gap increased to around $2 \times 10^{-2}$ cm.

• Improve the core optimisation process.

• Utilisation of a coupled 3D thermal-hydraulic, neutronic transient code to assess the behaviour of fuel rods during transient accidents such as rapid removal of RCCAs.

• Assess the benefits associated with enriched gadolinium burnable poison and/or investigate the $\lambda(T)$ and achievable densities for UO$_2$ fuel containing greater than or equal to 20 wt.% Gd$_2$O$_3$.

• Benchmarking of codes with UO$_2$ assemblies with enrichments between 5-20 wt.% in order to assess their ability in modelling epithermal LWR systems.

Secondary

• Screen potential Zr-based alloys that can be used as fuel cladding under CANDU water chemistry conditions.

• In order to eventually license a reactor core containing ultra-high burnup rods it will be necessary to assess the failure rate for such rods during power ramps. This data can then be used to improve PCI modelling of such fuel.

• Alternative poison mixtures as outlined in Section 6.4.1.

• Calculate the stresses the nuclear containment structure would potentially be exposed to, for instance during a collision with another ship. This information could then be used to assess precisely how robust the containment structure must be and the associated economic penalty of such a structure.

Other Potential Considerations

• Compare this core with one capable of achieving a 7.5 year core life. This could be used to assess the economic advantage of using a shorter core life, in particular with respect to enrichment and uranium utilisation costs. This is because as core life is extended, and enrichment and poison concentration increase, the spectrum hardens. Spectral hardening results in a poorer uranium utilisation as the benefit attached to increased $^{235}$U inventory diminishes. Hence by assessing
the economic detriment of higher enrichments and poison loadings this should then be used to analyse the economic benefit attached to a reduction in the number of fuel reloadings required.

- It is likely to prove difficult to design a PWR that is capable of total elimination of soluble boron, nevertheless, assessing the ability of alternative poison geometries and/or the incorporation of neutron absorbing sacrificial material to allow unborated water to be used in a core melt accident would also be worthwhile.
Appendix A

Emission Reduction Potential

A.1 Limits of Current Technology

In constructing Table 1.1 in Chapter 1 it was assumed that all electricity and heating were decarbonised, therefore emissions from buildings and all transport types besides ships and aircraft were set to zero (hence all vehicles and rail transport were electrified). It was also assumed that emissions related to deforestation no longer occurred. This effectively left emissions produced from shipping, air transport, food and industry.

A.1.1 Agriculture

Ref. [197] states that there is the potential to reduce agriculture emissions through a variety of efficiency mechanisms by around 50%, which was therefore used to reduce present agriculture emissions.

A.1.2 Air Transport

In the case of air transport the latest generation of aircraft are approaching fundamental limits in how much further they can improve their efficiency [6]. There are a number of radical alternatives such as solar powered aircraft and airships but currently they are incapable of replacing the capability of jet aeroplanes (namely their long range and high speeds) [4]. It is therefore concluded that current technology is unlikely to reduce the GHG intensity of air travel. In addition, hydrogen as a fuel for aircraft is also unsuitable, not least because its low volumetric energy density would increase the size
and weight of the aircraft resulting in a corresponding degradation of performance [4].

A.1.3 Shipping

The reductions assumed possible in shipping were outlined in Section 1.2 in Chapter 1. One means to reduce emissions from ships that was ignored, due to a variety of technical barriers, was utilising Carbon Capture and Storage (CCS) technology on board ships. This option has been mooted for use on large ships [25]. However, carbon capture devices reduce a power station’s efficiency by around 25% [6] and it is therefore likely ships would suffer a similar detrimental impact on fuel efficiency. The carbon capture system would also reduce the available space on board, as systems would need to be in place to process and store the carbon. The ships could then offload their inventory of CO$_2$ at predetermined locations where it would be pumped deep into the ocean.

At depths below 3000 metres the liquid CO$_2$ achieves a higher density than that of sea water, thus forming a ‘lake’ of CO$_2$ [46, 25]. However, besides the uncertainties surrounding the effects on marine life, there are considerable unknowns relating to storage reliability, with estimates varying from 30 years to 10,000 years depending on whether ocean currents disturb the settled CO$_2$ stream or the CO$_2$ very slowly dissolves into the sea water [46]. Hence, in the unlikely case CCS is implemented on board ships, it would probably be better to offload CO$_2$ at ports for final processing and storage.

A.1.4 Industry

Current industrial emissions are around 15.5 GtCO$_2$eq, with around 10.5 GtCO$_2$ attributable to energy usage (electricity and heating) [5]. Assuming heating and electricity are fully decarbonised and emissions from waste streams are reduced (currently around 1.5 GtCO$_2$eq) then process emissions are all that remain. It is very difficult to avoid these process emissions as they occur from the inherent chemical reactions that are required to produce the desired goods. Although in some cases, for example in hydrogen production, processes that utilise electrolysis may be able to significantly reduce emissions by utilising different chemical reactions to create the desired materials. However, as discussed in Section 1.2.2 in Chapter 1, there are significant energy inputs required to drive electrolysis reactions, hence the reason for its use only where absolutely necessary (e.g. in the case of aluminium production where no economic alternative has been found or very pure hydrogen gas is required). Therefore it was assumed that in the case of industrial process emissions there appear to be currently
limited technological means to cut these emissions by relying heavily on alternative low-greenhouse
gas emitting chemical processes. In fact, as the predominant GHG emitted by industrial processes is
CO$_2$, many industries are pursuing carbon capture and storage in preference to trying to find different
chemistry pathways for producing goods [46].

CCS will likely have to play some role in the future reduction of CO$_2$ emissions for the reasons
described above. However, it seems questionable to rely heavily on low-carbon emission reductions
from CCS, not least because the ability to robustly store CO$_2$ is uncertain. Currently, the only means
to store CO$_2$ at relatively low cost, with low environmental impact, and high confidence regarding
storage integrity, is using depleted oil and gas reservoirs. This is because a significant proportion of
the infrastructure is in place (wells and pipes), in addition to the host geology being well characterised.
However, given current CO$_2$ emissions, it appears unlikely that the maximum storage capacity achiev-
able from oil and gas reservoirs will be more than 700 GtCO$_2$ [46]. This would be sufficient to store
200 years worth of current industrial emissions (or around 20 years of global CO$_2$ emissions). If the
approximate 3.5 GtCO$_2$ of industrial process emissions were to be compressed to sufficient pressures
suitable for geological disposal in depleted oil and gas reservoirs then this would require a volume of
fluid to process of around 4.5 billion cubic metres, which is approximately the same volume of fluid
that the oil industry is able to process each year [46]. Therefore CCS, which is still very much in its
infancy, would need to be ramped up to a scale equivalent to the global oil industry which has taken
over a century to achieve, just to deal with industry process emissions.

A.2 Alternative Options

All of the options discussed in Section A.1 and in Chapter 1 have ignored the potential for demand
reduction, simply because demand reduction is much less popular than relying on technological means
to reduce emissions. Hence a series of bold assumptions were made regarding decarbonisation of land
transport, and the production of heat and electricity. Even factoring in these assumptions it appeared
likely that many radical breakthroughs would need to be made in the areas of flying, numerous
industrial processes, shipping and food production to limit GHG emissions so that temperatures rises
in excess of around 2°C are unlikely to occur. The probability that all of these will take place seems
low and therefore some form of demand reduction will likely be necessary to reduce GHG emissions.

Strategies based on increasing the intensity of use and life extension of various machines and
structures, along with reductions in consumer waste, could offer considerable emission reductions [46]. For instance, buildings and infrastructure - which both are high consumers of CO₂ intensive steel and cement - contain core structural materials that can last for over 200 years if adequately maintained [5]. However, their current typical lifetimes are less than 80 years [5]. Furthermore many household goods can in principle be designed to last for life assuming repairability is placed at the forefront when designing the products [46]. Therefore, as a large proportion of global shipping is responsible for transporting many of these goods, any reduction in the use of these goods would have corresponding reductions in emission rates from ships.
Appendix B

Uranium Core

B.1 Practical Considerations Relating to High-Gadolinia Fuel

Data was gathered relating to the material characteristics of high-gadolinia doped fuel. These are summarised below.

Thermal Conductivity

In oxide fuel, of all the various material characteristics - including achievable density through sintering, elastic modulus and melting point - one of the most important from a fuel performance perspective is the material’s thermal conductivity [126]. Figure B.1 shows the degradation of thermal conductivity as a function of gadolinia content and temperature. There did not appear to be any data related to thermal conductivity as a function of temperature for fuels with gadolinia concentrations above approximately 15 wt.%. 
Typically fuel rods in conventional reactors have centreline temperatures of around 1000°C, therefore, from Figure B.1, at such temperatures thermal conductivity degrades by around 15% in the case of gadolinium doped fuel with around 14 wt.% Gd$_2$O$_3$ relative to undoped fuel [198].

**Achievable Densities**

Another property of interest is the material’s density, primarily due to its impact on the achievable uranium densities, which impact fuel cycle lengths for a given $^{235}$U enrichment. Reported data on achievable densities at very high gadolinia concentrations (up to 30 wt.%), through sintering processes comparable to those carried out in conventional pellet fabrication, are in the range 94-96% of theoretical density [135]. These are comparable to the density variation in low gadolinia content fuel [136]. Considering these two primary characteristics (thermal conductivity and fuel density), there did not appear to be any major barriers regarding the use of fuels containing very high gadolinia concentrations based on the published data.

**Additional Material Characteristics**

Besides achievable densities through conventional fabrication routes and thermal conductivity behaviour of high gadolinia fuel, pellets containing up to 30 wt.% gadolinia have also been heated up to peak temperatures of 2100°C, in order to study the thermal migration of gadolinium [135]. If gadolinium was found to migrate under thermal gradients thus causing considerable changes in fuel properties due to the depletion/accumulation of gadolinium, this would complicate modelling of the
fuel and may result in physical processes that make the fuel unsuitable for use in a reactor. For example, if it was found that gadolinium tended to concentrate in higher temperature regions and knowing that gadolinium tends to degrade the thermal conductivity of UO$_2$ fuel, this could lead to an increase in temperature and greater accumulation of gadolinium, a positive feedback phenomenon could therefore ensue. However, experiments (over a 100 hour period) resulted in no detectable thermal migration of gadolinium [135]. Experiments on the elastic modulus showed that it was virtually unaffected at gadolinia concentrations up to 20 wt.\% [136]. The effects of gadolinia concentration on melting temperature of (U,Gd)O$_2$ fuel has been investigated up to 25 wt.\%, with reductions in melting temperature of around 60°C observed, which is relatively small given the melting point of UO$_2$ fuel is around 2800°C [136].

Issues relating to the back-end of the fuel cycle are also deemed to be very small, especially in comparison with other issues relating to the higher proportion of minor actinides, plutonium and fission products within the high burnup fuel [52]. Gadolinium is frequently added to the dissolver of a reprocessing plant to increase the margin to criticality and Gd has also been proven not to interfere with the chemistry of the process (it is readily recovered in the High Level Waste (HLW) stream and subsequently vitrified). Although given that gadolinia contributes to oxide loading, there will be the downside of increasing the volume of vitrified waste [136]. Finally, if the considerable fissile material within the spent fuel is deemed uneconomic to reprocess then higher Gd$_2$O$_3$ doped fuel has been shown to have lower dissolution rates than undoped fuel. Although it appears that at levels greater than 4 wt.\% in un-irradiated fuel the dissolution rate levels off [199].
B.2 Sample of Colourset Models

Figure B.2: Sample of some of the colourset models runs that were used for deciding on the appropriate lattices to achieve the desired reactivity profile. The above core results all consist of lattices containing 76 and 48 burnable poison pins.

Figure B.3: Sample of some of the colourset models runs that were used for deciding on the appropriate lattices to achieve the desired reactivity profile. The above core results all consist of lattices containing 96 and 76 burnable poison pins.
B.3 Axially Homogeneous Rod Insertion

Figure B.4: Dependence of RCCA position as a function of core life for the core prior to axially varying the poison and enrichment concentrations. This core employs the 45 RCCA layout shown in Figure 3.10a. Without axially varying the poison and enrichment concentrations, the RCCA penetrations throughout life are relatively deep (> 50% of the way into the active region of the core).

B.4 Power Profile

Figure B.5: Radial slice through row 6 of the axially homogeneous core at various points in time, with no RCCAs inserted. This illustrates the evolution of the power profile throughout core life without the RCCAs inserted.
B.5 Individual assembly burnup histories

Figure B.6: Histogram of the rod burnups for the assemblies in one octant of the core. The blue histograms indicate burnup histories for burnable poison pins, whereas the transparent histograms indicate the burnup histories for the fuel pins (containing no burnable poison).

B.6 Core Reactivity After Shutdown

As the ship will have to call into a port at various points in its life, the time dependence of a shutdown reactor is clearly of interest. Once the reactor is shut down there are many nuclides that contribute...
significantly to reactivity behaviour besides $^{135}$Xe and $^{135}$I. Table B.1 lists the most important nuclides along with their half-lives and impact on core reactivity, namely the addition or removal of neutron absorbing nuclides and/or the addition or removal of fissile nuclides.

<table>
<thead>
<tr>
<th>Parent Nuclide</th>
<th>Daughter</th>
<th>Half-life</th>
<th>Impact</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{135}$I</td>
<td>$^{135}$Xe</td>
<td>6.6 h</td>
<td>+absorber</td>
</tr>
<tr>
<td>$^{135}$Xe</td>
<td>$^{135}$Cs</td>
<td>9.2 h</td>
<td>-absorber</td>
</tr>
<tr>
<td>$^{145}$Pm</td>
<td>$^{147}$Sm</td>
<td>2.2 d</td>
<td>+absorber</td>
</tr>
<tr>
<td>$^{239}$Np</td>
<td>$^{239}$Pu</td>
<td>2.4 d</td>
<td>+fissile</td>
</tr>
<tr>
<td>$^{148}$Pm</td>
<td>$^{148}$Sm</td>
<td>5.4 d</td>
<td>-absorber</td>
</tr>
<tr>
<td>$^{148m}$Pm</td>
<td>$^{148}$Sm</td>
<td>41 d</td>
<td>-absorber</td>
</tr>
<tr>
<td>$^{155}$Eu</td>
<td>$^{155}$Gd</td>
<td>4.7 y</td>
<td>+absorber</td>
</tr>
<tr>
<td>$^{241}$Pu</td>
<td>$^{241}$Am</td>
<td>14.4 y</td>
<td>-fissile/+absorber</td>
</tr>
</tbody>
</table>

Table B.1: Nuclides that impact reactivity behaviour once a reactor is shut down - divided into short-, medium- and long-term impact.

Figure B.7 shows the time dependence of $k_{eff}$ at various core life intervals after 81 RCCAs have been inserted and core inlet temperature set to 20°C. In all cases there is an increase in reactivity of up to around 1000 pcm over the course of around 4000 hours (170 days), with the majority of the reactivity increase occurring over the first 100 hours. This was attributed to the decay of $^{148}$Pm, which has a thermal absorption cross-section of around 2000 barns vs around 3 barns for $^{148}$Sm and the decay of $^{239}$Np to fissile $^{239}$Pu.
Figure B.7: Core reactivity once shutdown has occurred at various points in core life.

B.7 Reactivity Coefficients

Figures B.8 and B.9 show the very limited dependence of Moderator Temperature Coefficient (MTC) and Distributed Doppler Coefficient (DDC) on fission product inventory treatment at Cold Zero Power (CZP) and Warm Zero Power (WZP) conditions.

Two types of fission product treatment were studied, which were no change in xenon and iodine concentrations ([Xe] and [I]) from their concentrations prior to the transient, and the xenon and iodine concentrations set to zero. The latter assumes sufficient time has passed that the inventory of these nuclides will have completely decayed away.
Figure B.8: Dependence of Moderator Temperature Coefficient as a function of core life on fission product inventory treatment at Cold Zero Power and Warm Zero Power, which correspond to coolant inlet temperatures of 20°C and 100°C respectively.

Figure B.9: Dependence of Distributed Doppler Coefficient as a function of core life on fission product inventory treatment at Cold Zero Power and Warm Zero Power, which correspond to coolant inlet temperatures of 20°C and 100°C respectively.
Figures B.10 and B.11 show the behaviour of MTC and DDC under a variety of reactor states. These states include CZP and WZP at Critical Rod Positions (CRP), which corresponds to the reactor state with control rod banks withdrawn to a height that produces a $k_{\text{eff}}$ of 1.0000 (with a convergence tolerance of 0.0025) and which preserves the bank order, i.e. control bank 4 removed first, followed by bank 3, then bank 2 and finally bank 1, resulting in bank 1 always at the greatest penetration. In addition, the reactor state Hot Partial Power (HPP), which was taken to correspond to the reactor operating at 25% of the rated core power, i.e. 110 MWth, was also investigated. This latter state would likely be the approximate power of the marine reactor when it has entered port and is only meeting the hotel load of the ship. As can be seen, all of the coefficients are negative under all of the states studied.

![Moderator Temperature Coefficient behaviour](image)

Figure B.10: Moderator Temperature Coefficient behaviour in a variety of reactor states, including Hot Partial Power (HPP) and Critical Rod Positions (CRP). The former corresponds to the core running at 25% of rated power (110 MWth) and the latter is the reactor state when banks have been moved to ensure $k_{\text{eff}}$ of 1.0000 with a convergence tolerance of 0.0025.
B.8 Xenon Fission Product Effects

Figure B.12 shows the behaviour of $^{135}$I and $^{135}$Xe under HZP conditions from the onset of shutdown ($t = 0$ hours). As can be seen, the difference between equilibrium and peak xenon is minimal in all cases.
Figure B.12: Evolution of $^{135}$I [I] and $^{135}$Xe [Xe] concentrations at various points in core life.
B.9 Benchmarking with MONK

B.9.1 Time Step Sensitivity

Figure B.13: Sensitivity of burnup run to time step. Time step 1 consisted of steps of 0.25 days up to 2 days and then progressed in time steps of 12.5 days up to 77 days and subsequent steps were 35 days. Time step 2 also consisted of 0.25 day steps up to 2 days and then progressed in steps of 6.25 days up to 77 days and the remaining steps were 17.5 days. No change was made to the initial time step of 0.25 days as a sensitivity study found this was sufficient to model the initial buildup of xenon in the core.

B.9.2 Axial Region Size Sensitivity

As the core consists of 16 unique assemblies (which describe an octant of the core) and there are 2 distinct rod types per assembly (burnable poison pins and non-burnable poison (fuel) pins), this results in requiring the 32 materials to record the radial burnup history. Note that using a single distinct region for the burnable poison pins, and another for the fuel pins, results in the burnup being averaged across all fuel pins in an assembly; the same is true for burnable poison pins, but given the size of each assembly (21.42 cm by 21.42 cm) vs the whole core size (diameter equal to 245.14 cm) this was believed to be an acceptable approximation for recording fairly accurately the effect of burnup on $k_{\text{eff}}$. Each assembly was then split into a number of axial regions, so in the case of 9 axial regions there were in total 288 regions to describe the radial and axial burnup of the entire core. Figure B.14 shows the sensitivity of the MONK depletion results to the number of axial regions.
Figure B.14: Sensitivity of the MONK depletion results to number of axial regions.

With 6 axial regions to store the individual nuclide inventory content as a function of time, the \( k_{\text{eff}} \) evolution diverges by quite a considerable margin relative to the results for 9 and 12 axial regions. Clearly 6 axial regions were not sufficient whereas the difference between the 9 and 12 axial region runs was judged sufficiently small to permit models based on 9 axial regions to be used without any significant bias introduced by the lower model fidelity.
B.10 Axial Offset for Isothermal Core Run

![Graph showing Axial Offset over Time](image)

Figure B.15: Axial offset as a function of time for core operating under isothermal conditions ($T_{\text{inlet}} = T_{\text{outlet}} = T_{\text{fuel}} = 255^\circ\text{C}$).

B.11 Flux Distribution for Different Lattices

Figure B.16 shows the flux distributions predicted by CASMO-4 for Cases 1A and 3A in Table 3.6. Note that besides the large differences in flux distribution at thermal energies, above approximately 100 eV, the spectra also start to diverge by quite a large margin and in the $^{238}\text{U}$ fission threshold region (around 1 MeV) the fluxes diverge.
B.12 Fuel Performance Analysis of Rods E6-0611 and C8-1610

Figure B.17 shows the difference in burnup distribution between rods E6-0611 and C8-1610 that have very similar average burnups along the length of each rod. As can be seen, rod C8-1610 experiences much higher peak burnups, in particular axial zones 11 and 12 are significantly higher than any zones for rod E6-0611. Both rods contained solid pellets, a plenum length of 25.40 cm and a pellet-clad gap of 0.0205 cm.

It was found that the maximum clad hoop creep strain for rod C8-1610 was in zone 11.
B.18 shows the clad hoop creep strain for zones 11 and 12 for rod C8-1610 as a function of time. Whilst zone 12 has a slightly higher burnup than zone 11 (see Figure B.17) it was the case that zone 11 had a significantly higher clad surface temperature for the majority of its life in comparison to zone 12; in addition zone 11 had a higher fuel temperature early in its life. Therefore the overall effect was for the pellet-clad gap to close sooner in zone 11 compared to zone 12, and the clad hoop creep strain to be marginally higher in the slightly lower burnup zone.

Hence whilst achieving the highest burnup does not guarantee that an individual zone will be the most limiting with respect to various fuel performance criteria, it is a very good indicator when all other phenomena are effectively equal.
There is currently limited data on the behaviour of ultra-high burnup UO$_2$ fuel rods in Zirconium-based alloy clad operating in LWRs, especially up to the peak burnup in the current core design (around 120 GW.d/tHM using solid pellets), which could be used as a proxy for fuel rods in the marine reactor core studied here. However, Siemens have previously examined the behaviour of rods operating in PWRs up to an average end of life burnup of 98 GW.d/tHM, residing in the reactor core for 9 cycles (around 9 years). Figure B.19 compares the linear ratings reported for the rods in Siemens' high burnup study [39]. Note that in Ref. [39] the linear ratings reported are based on the largest average linear rating calculated for a particular rod during each of its cycles. Therefore Figure B.19 displays these 9 data points, in addition to 2 extra data points that are based on linearly extrapolating neighbouring data points in order to approximately determine the rating at the beginning and end of rod life.

Figure B.19 not only displays the average linear rating from the peak burnup rod from the marine reactor at time steps (0, 2.5, 5, 7.5, 10, 12.5 and 15 years), but also includes the peak axial rating for this rod at each of these time steps. This was to account for the skewed axial profile in the soluble boron free reactor design, which results in rod segment power ratings deviating considerably from the mean rating.
Whilst the high burnup rods in the Siemens study do not experience typical irradiation histories for rods operating in a commercial reactor throughout life, they do appear to show a similar ratings profile to the high burnup rod in the marine reactor. Towards the end of life in the marine reactor, the high burnup rod does unfortunately experience an increase in maximum linear rating as the control rods are fully removed. This not only results in a departure from the similarity of the rating profiles, but also increases the rod power at the very point when the rod is extremely sensitive to increases in rod power due to it having very high burnups. Furthermore, although the high burnup study rods experience a higher mean rating over the course of their lives (21 kW/m vs 11 kW/m), the rods in the marine reactor reside in the core for a significantly longer period of time and their pellet diameters, whilst relatively large in comparison to standard pellet dimensions, are significantly thinner than the pellets in the Siemens study (0.465 cm vs 0.4267 cm). Nevertheless, it appears sensible to consider basing targeted peak burnups to less than 98 GW.d/tHM in future studies, as data is available to support the feasibility of operating rods up to this level under LWR conditions with similar ratings profiles to the peak burnup rods in the marine reactor core. However, the scarcity of data on fuel rods experiencing relatively frequent power ramping at very high burnups (in excess of 60 GW.d/tHM), in particular relating to PCI performance, would need to be addressed before it is possible to pronounce with any degree of confidence on the suitability of ultra-high burnup rods employing UO$_2$ pellets in a zirconium-based clad for use in marine propulsion.

**B.14 Dual Cooled Fuels**

Given that annular pellets have been investigated in order to reduce rod internal pressure and to limit the stresses applied to the cladding material due to pellet swelling, and the fact that various fuel degradation mechanisms (such as Pellet Clad Interaction) are heavily dependent on the fuel temperature, it is tempting to suggest that the rod is internally cooled to reduce the fuel temperature further. However, in reality the internal cooling volume must be optimised in order to ensure sufficient coolant passes through the centre of the fuel in order to benefit from the advantages attached to internally cooled fuels [198]. This results in a considerably different rod geometry as the overall pellet size is increased and hence the overall rod diameter is increased from around 0.95 cm to around 1.54 cm [198]. This does not permit these rods to be used in conventional grid spacers.

Interest in Dual Cooled Fuels (DCF$s$) is focused primarily on reducing the amount of stored heat
in the fuel, which is beneficial during accident scenarios where impaired cooling makes removing heat more difficult, or using the improved safety performance of DCFs to raise the power density of the core in order to extract more power from a given core size [198]. There does not appear to be any data regarding the ability of internal cooling to alleviate the issues relating to ultra-high burnups, such as the increased fission gas release and the larger extent of fuel swelling as a function of burnup.

Annular fuel pellets without any internal cooling appear in themselves an effective strategy without the need to radically alter the rod geometry and avoid issues relating to blockages from debris that may limit coolant propagation through the centre of DCFs. There is also the greater surface area of chemically reactive zirconium in DCFs that could increase the amount of hydrogen produced in the event of a failure in the core cooling system. Therefore, if it is the case that further core optimisation cannot reduce the maximum rod burnups and therefore requires the use of annular pellets, it appears sensible to focus on non-internally cooled geometries over DCFs.

B.15 Behaviour of Clad Hoop Creep as a Function of Clad Surface Temperature

Table 3.10 shows some examples where - as the channel mass flow rate is reduced, and therefore clad temperature increases - the maximum clad hoop creep strain in some instances is reduced. For example, rod D7-0204 had a maximum clad hoop creep strain of 0.39% when the flow rate was fixed to 290 g.s$^{-1}$, yet when the flow rate was reduced by approximately half to 150 g.s$^{-1}$ the maximum clad hoop creep strain reduces to 0.36%. Creep is defined as time-dependent plasticity that arises due to mechanical stresses applied to a solid material, for example the forces exerted on the clad from the high coolant pressure. There are several mechanisms that contribute to creep, including the movement of dislocations in the lattice, the diffusion of atoms through grains and the diffusion of atoms along grain boundaries. All of these diffusional processes have in general a strong temperature dependence [200].

Typically in nuclear fuel, as a rod’s surface temperature increases its end of life clad hoop creep strain becomes relatively large and positive. Therefore rods that operate at high surface temperatures (low mass flow rates) but experience lower maximum clad hoop creep strain values are unusual. Analysing rod D7-0204 it was found that in the two cases run - one with a high mass flow rate and

---

$^{1}$Dislocation creep is dependent upon the diffusion of vacancies.
the other with a lower mass flow rate - the maximum clad hoop creep strain over the rod's histories occurred in axial zone 6. Figure B.20 shows the time dependence of the clad surface temperature within this region as a function of mass flow rate. Unsurprisingly the lower mass flow rate results in a higher clad outer surface temperature.

Figure B.21 shows the clad hoop stress as a function of time in this zone for the two mass flow rates investigated in axial zone 6 of rod D7-0204. It turns out to be the case that as there is a relatively large pellet-clad gap in the rods (to accommodate the pellet swelling that occurs inside the rods), the initial creep is inwards due to the external pressure of the coolant. Therefore, as this initial creep is temperature dependent, the higher clad temperature in the low mass flow rate case results in a greater amount of inward creep and then by the time pellet swelling starts to dominate, the outward creep rate is not sufficiently large to overcome the initial amount of inward creep, and hence the clad hoop creep strain at the end of life is smaller than the low temperature case.

![Clad surface temperature over core life as a function of channel mass flow rate for axial zone 6 out of 16 in fuel rod D7-0204.](image)

Figure B.20: Clad surface temperature over core life as a function of channel mass flow rate for axial zone 6 out of 16 in fuel rod D7-0204.
Figure B.21: Clad hoop creep strain over core life as a function of channel mass flow rate for axial zone 6 out of 16 in fuel rod D7-0204.

Note that the clad surface temperature decreases by quite a significant amount over the course of its life because the power within any rod section changes quite dramatically as the control rod’s position changes and thus the local rod power peak moves from one region to another.
Appendix C

Thorium Core

C.1 Core Reactivity After Shutdown

Figure C.1 shows the reactivity change over an extended period of time (>1000 hours) under cold zero power conditions. The largest reactivity increase occurred at \( t = 15 \) years and was slightly higher than the UO\(_2\) core case. This was attributed to the greater inventory of \(^{233}\)Pa, which has a relatively long half-life and decays to fissile \(^{233}\)U.

Figure C.1: Reactivity change once shutdown has occurred and core coolant temperature has reached 20° C (Cold Zero power conditions).

\[ 10 \text{ days} \quad 5 \text{ years} \quad 10 \text{ years} \quad 15 \text{ years} \]

\[ k_{\text{eff}} \quad 0.83 \quad 0.84 \quad 0.85 \quad 0.86 \quad 0.87 \]

\[ \text{Time (Hours)} \]

\[ 0 \quad 1000 \quad 2000 \quad 3000 \quad 4000 \quad 5000 \]
Appendix D

Details of $^{232}\text{Th}/^{233}\text{U}$ Benchmark Models Investigated
Figure D.1: Core configurations for LEU (2 wt.% $^{235}$U) fuelled cores with no thorium present in any of the channels. The original core names from Ref. [37] are included in brackets. The black, white, red and blue circles indicate detector, empty, unflooded fuel and flooded fuel channels. The light and dark green blocks indicate reflector and core graphite respectively.
Figure D.2: Core configurations for cores with LEU (2 wt.% $^{235}$U) fuel channels and thorium channels. The original core names from Ref. [37] are included in brackets. The black, white, red and blue circles indicate detector, empty, unflooded fuel and flooded fuel channels respectively. The light and dark green blocks indicate reflector and core graphite respectively. The yellow and green circles indicate unflooded and flooded thorium channels respectively.
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